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NUREG/CR-4161
UCID-20092
Vol. 2

Critical Parameters for a High-Level Waste Repository

Volume 2: Tuff

E. P. Binnall, S. M. Benson, L. Tsao, H. A. Wollenberg, T. K. Tokunaga, and E. M. Didwall

Prepared for
U.S. Nuclear Regulatory Commission

Lawrence
Livermore
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NUREG/CR-4161
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RW

Critical Parameters for a High-Level Waste Repository
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Manuscript Completed: February 1987
Date Published: May 1987

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ABSTRACT

This report addresses critical parameters specific to a repository in tuff, using the Topopah Springs Member of the Yucca Mountain tuffs as the principal example. For the purposes of this report, a parameter is considered to be a physical property whose value helps determine the characteristics or behavior of a repository system. Parameters which are defined as critical are those essential to evaluate and/or monitor leakage of radionuclides from the repository and to evaluate the need for retrieval. The parameters are considered with respect to the disciplines of geomechanics, geology, hydrology, and geochemistry, and are rank ordered in terms of importance. The specific role of each parameter, specific factors affecting the measurement of each parameter, and the interrelationships of the parameters are considered. Diffusive transport of gaseous radionuclides through the unsaturated zone of fractured porous media is given special attention in the Appendix.

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CONTENTS

ABSTRACT iii

LIST OF FIGURES vii

LIST OF TABLES vii

ACKNOWLEDGMENTS ix

NOMENCLATURE xi

EXECUTIVE SUMMARY 1

1.0 INTRODUCTION 2

2.0 CRITICAL PARAMETERS FOR TUFF 3

3.0 DETAILED CRITICAL PARAMETER CONSIDERATIONS 13

3.1 Geomechanical Parameters 13

3.1.1 Displacement and Deformation 13
3.1.2 Fracture Properties and Induced Fractures 15
3.1.3 Initial *In Situ* Stress and Stress Changes 17
3.1.4 Rock Strength 19
3.1.5 Rock Modulus and Poisson's Ratio 21
3.1.6 Temperature 24
3.1.7 Expansivity 27
3.1.8 Thermal Conductivity, Heat Capacity, and Diffusivity 30
3.1.9 Convective Heat Transfer 33
3.1.10 Decrepitation and Spalling 37
3.1.11 Canister Movement 39

3.2 Geologic Parameters 41

3.2.1 Crustal Deformation 42
3.2.2 Naturally Occurring Radionuclides 42
3.2.3 Seismicity 43
3.2.4 Lithologic Parameters 44
3.2.5 Faulting 45
3.2.6 Folding 45
3.2.7 Erosion Rate 45
3.2.8 Water, Mineral, and Petroleum Resources 45
3.2.9 Potential Igneous Activity 45

3.3 Hydrologic Parameters 45

3.3.1 Hydrostratigraphic Units 46
3.3.2 Permeability (Fracture and Matrix) 47
3.3.3 Relative Permeability 49
3.3.4 Water Saturation 51
3.3.5 Porosity and Distribution of Pore Sizes 52
3.3.6 Saturation Characteristic Curve 54

3.3.7 Water Potential 56
3.3.8 Water Infiltration Rate 58
3.3.9 Water Inflow Rate 59
3.3.10 Fluid Velocity 60
3.3.11 Groundwater Recharge and Discharge 61
3.3.12 Seal and Backfill Properties 62

3.4 Geochemical Parameters 62

3.4.1 Groundwater Chemistry 63
3.4.2 Age of Water 65
3.4.3 Sorptive Capacity of Formation Rock 66
3.4.4 Solubility of Radionuclides of Interest 66
3.4.5 Volatility and Gaseous Diffusion of Radionuclide Chemical Species 68
3.4.6 Canister and Support System Corrosion 70
3.4.7 Radionuclide Leakage Rate 72
3.4.8 Seal and Backfill Leakage 73

4.0 CONCLUSIONS 74

REFERENCES 77

APPENDIX. DIFFUSIVE TRANSPORT OF GASEOUS RADIONUCLIDES .... A-i

LIST OF FIGURES

1. Critical parameter time line for a repository in tuff 4

LIST OF TABLES

1. Prioritized critical parameters for site characterization, tuff 5
2. Prioritized critical parameters for site construction, tuff 6
3. Prioritized critical parameters for site operation, tuff 7
4. Prioritized critical parameters for site closure, tuff 8
5. Prioritized critical parameters by discipline for site characterization, tuff 9
6. Prioritized critical parameters by discipline for site construction, tuff 10
7. Prioritized critical parameters by discipline for site operation, tuff 11
8. Prioritized critical parameters by discipline for site closure, tuff 12
9. Near-field *in situ* stresses in Yucca Mountain tuffs 18
10. Summary of rock strength parameters for Topopah Springs tuff 20
11. Comparative values of Young's modulus and Poisson's ratio for Yucca Mountain tuffs 23
12. Linear thermal expansion coefficients from 21 samples of devitrified welded tuff 28
13. Thermal expansions coefficients of Yucca Mountain tuffs 29
14. Thermal parameters and associated physical properties of Yucca Mountain tuffs 32
15. Calculated heat capacities for saturated and dry tuff rock masses as a function of porosity and grain density 32
16. Boiling points of candidate radionuclides for gas-phase transport 69
A.1. Some proposed forms of $f(\phi_g)$ A-5

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ACKNOWLEDGMENTS

The authors are grateful for program guidance by the late Dr. Jeff Lytle of the Lawrence Livermore National Laboratory, which he provided even through difficult periods of his long fight with cancer. We miss his friendship and support.

We wish to express our appreciation to Jeff Braithwaite, Brenda Langkopf, and Roger Zimmerman of Sandia National Laboratories for their informal discussion with us on critical parameter measurements for a repository in tuff. We are especially grateful to Prof. Stanley N. Davis of the University of Arizona for his communications on the age dating of water, to Larry Perrine of SNL for his efforts in supplying many of the technical reports used as references in preparing this report, and to Ernst Zurflueh of the U.S. Nuclear Regulatory Commission for his support of this project.

We also thank Stephen Greenberg of LLNL for his careful editing, and Pat Johnston and Jean Wolslegel of the Lawrence Berkeley Laboratory for their word processing and final preparation of this report.

Prepared for Division of Radiation Programs and Earth Sciences, Office of Nuclear Regulatory Research, U.S. Nuclear Regulatory Commission, Washington, DC 20555, under Interagency Agreement DOE, NRC FIN No. A0367, through U.S. Department of Energy Contract Numbers DE-AC03-76SF00098 with Lawrence Berkeley Laboratory and W-7405-ENG-48 with Lawrence Livermore National Laboratory.

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NOMENCLATURE

List of Abbreviations

AE	acoustic emission
BWIP	Basalt Waste Isolation Project (Hanford, Washington)
CHLW	Commercial high-level waste
DOE	U.S. Department of Energy
GTL	gross thermal loading
HLW	high-level waste (includes spent fuel for this report)
LBL	Lawrence Berkeley Laboratory
LLNL	Lawrence Livermore National Laboratory
NRC	U.S. Nuclear Regulatory Commission
NTS	Nevada Test Site
ppm	parts per million
SAC	Swedish American Cooperative (Project at Stripa, Sweden)
SNL	Sandia National Laboratories
TC	thermocouple
USGS	United States Geological Survey

EXECUTIVE SUMMARY

As a task in the evaluation of geotechnical, environmental, and radiation field measurement systems for nuclear waste isolation, geomechanical, geologic, hydrologic, and geochemical parameters critical to emplacement of radioactive waste in tuff have been identified. For purposes of this report, a parameter is considered to be a physical property whose value helps determine the characteristics or behavior of a repository system.

The parameters have been chiefly addressed using the geologic setting of the Yucca Mountain tuffs at or bordering the Nevada Test Site with special emphasis on the unsaturated, devitrified, welded tuff of the Topopah Springs Member.

Of strongest consideration were measurements that focused ultimately on the contamination by radionuclides of water that could become accessible to the biosphere. In this respect, direct assumptions were not made concerning probable radionuclide pathways. Rather, measurements were considered that would be used to evaluate essentially all potential pathways between the repository and, ultimately, the surface.

In this assessment, a parameter is considered to be "critical" if a mistake in its measurement, or the inability to measure it, could lead to the wrong conclusions about the adequacy of a repository. The phase of development of a repository is important in considering the criticality of a parameter. A parameter is critical only during the phase or phases when it must be measured or monitored. Once a parameter has been determined and is considered to be nonvarying, it is no longer considered critical for measurement or monitoring purposes.

The relative importance of critical parameters for tuff was determined for each phase of repository activity: site characterization, construction, operation (including retrievability), and closure and decommissioning. Figure 1 lists parameters and shows their time sequence during repository phases. These phases are not necessarily distinct time periods, but may overlap each other. For example, operations may start in one underground location well before construction is completed in another sector of the repository.

The relative ranking of closely spaced (in importance) parameters is only approximate and can change significantly, depending on site-specific considerations and on the increased understanding of each parameter's importance. Even though the rank ordering is somewhat subjective and can change with future information, the magnitude of each change will probably not be great. The exact priority of each parameter is considered less important than having the critical parameters clearly defined.

Priorities were assigned to critical parameters for each phase, as indicated in Fig. 1, and are tabulated and described in detail by discipline (geomechanics, geology, hydrology, geochemistry) in the body of the text. Of greatest concern in the site characterization phase is establishing an understanding of the geologic setting, especially the depth, thickness, orientation, and lateral continuity of hydrostratigraphic units encompassing and bounding the proposed repository rock mass. An understanding of the hydrologic characteristics of these hydrostratigraphic units is also of principal concern during the site characterization phase, with monitoring of these parameters continuing into subsequent phases. Measurements of the age of water, and the sorptive capacity of rock matrix and fracture lining materials are geochemical parameters of primary importance during the site characterization phase. These are closely followed in importance by measurements to determine: groundwater chemistry; solubility, volatility, and gaseous diffusion of radionuclide species of interest; and canister and support system corrosion rates. The canister corrosion tests should be started during the site characterization phase and long-term observations conducted throughout the entire repository sequence. Characterization of the lithophysal, fracture, thermal, thermomechanical and mechanical properties of the rock mass is also of high priority during site characterization.

During the site construction phase, deformations and displacements, *in situ* stress changes, and induced fracturing will be major concerns as the underground construction progresses through the rock mass. As the construction proceeds, new openings will provide access for additional measurements of important critical parameters that may vary through the rock mass, such as: water potential, degree of water saturation of the rock, age of water, geologic variables, fracture properties, rock strength, variations in virgin *in situ* stress, variations in rock modulus and Poisson's ratio, and tectonic factors.

Highest-priority critical parameters during the site operation phase include those concerned with the response of the rock mass and hydrologic system to thermal effects from the introduction of radioactive waste. Critical parameters requiring measurement and long-term monitoring systems, installed during operations and extending into (and in some cases beyond) the closure and decommissioning phase of the repository, include as high priority those concerned with radionuclide leakage and the effectiveness of backfill and sealing systems.

Several geologic parameters, such as faulting, folding, and erosion rate, are not directly measurable by instrumentation systems, but may be determined indirectly by surface and/or subsurface geophysical techniques. Similarly, not all hydrologic parameters are directly measurable, but rely on interpretation of measurements of specific hydrologic properties of the rock mass.

In several cases, parameters will initially be measured in test facilities that will begin operation during the site characterization phase. The most important tests will monitor the performance of canisters, backfill and seals, and the hydro-thermo-mechanical response of the rock mass to the introduction of the waste. These measurements and long-term monitoring will subsequently be extended to the actual repository locations as canisters are emplaced, and as the repository sealing systems are established.

1.0 INTRODUCTION

This report is the second in a series (Binnall *et al.*, 1985) that covers an important identification phase for our current project whose objective is to consider the adequacy and reliability of the different measurement techniques and instruments which might be used by the DOE in the national high-level nuclear waste (HLW) disposal program. The repository phases of concern in the HLW program include site characterization, site construction, site operation, and closure and decommissioning. The measurements considered include all those which are used to characterize the site and/or to monitor the site performance and which will be used in the prediction of site performance adequacy for safe, long-term disposal of nuclear waste.

An important phase of the analysis of these measurements is an understanding of what must be measured and the special needs, if any, with respect to determining those parameter values. Numerous analyses have been performed in this regard, but have not resulted in a consensus regarding which parameters are critical, nor an estimate of the relative importance of the different parameters. Any consideration of the adequacy of an overall approach to parameter measurements must take into account these factors to assure that proper consideration be given to the most critical parameters. One reason that such a consensus does not presently exist is that media-specific and site-specific characteristics must be considered. In this report, we develop the critical parameter information for tuff, and consider site-specific information which allows us to address these parameters using the Yucca Mountain tuffs at, or bordering, the Nevada Test Site as examples (emphasizing the unsaturated, devitrified, welded tuff of the Topopah Springs Member).

Relatively few assumptions have been made regarding the specific pathways for release of radionuclides. For this study, we considered the possibility of contamination of subsurface water, which may eventually be accessible to the biosphere, to be a primary concern. Considerations pertinent to this concern include:

- canister failure due to corrosion and/or stress field encountered during storage,
- leaching of radionuclides from the waste form,
- radionuclide escape through package and backfill material, and
- radionuclide escape through the fractured, porous tuff.

We have not considered in detail: release of radionuclides that might accompany volcanic or seismic events, inadvertent human intrusion, or extensive surface erosion. Such possible release scenarios are largely determined on the basis of noninstrumented evaluations (*e.g.*, evidence of past volcanic or seismic activity or the presence of valuable mineral resources). With regard to contamination of accessible aquifers, no direct assumptions were made concerning probable pathways. Rather, we considered measurements which will likely be used to evaluate essentially all potential paths of communication between the repository and subsurface aquifers or ground surface.

In this study, we have not assumed nor proposed a particular methodology of site characterization or assessment. Instead, we have examined all of the physical properties and processes which may have bearing on the ability of a site to isolate radioactive waste and have chosen those which seem to be most significant, regardless of their compatibility with any specified assessment methodology.

Our definition of a critical parameter also needs to be considered. We consider a parameter to be critical if its mismeasurement could lead to incorrect conclusions regarding repository adequacy. The concept of mismeasurement in this case includes the inability to make a measurement. When the latter condition occurs, it is necessary to either measure additional alternative parameters which would result in reaching the correct conclusion concerning repository adequacy, or else a means must be found for evaluating the parameter in question. Often, these alternative parameters may not involve instrumentation but, rather, interpretation. In terms of prioritization, a parameter is considered to be less critical if, by not measuring it, the likelihood of drawing the wrong conclusion concerning repository adequacy is not increased. Hence, it can be concluded that a parameter is considered critical only during those repository phases when it must be measured or otherwise determined or monitored. Though knowledge of a parameter's values may be critical during repository phases following its determination, once the parameter has been determined and can also be considered as nonvarying, it is no longer considered critical for measurement or monitoring purposes.

In considering the likely values and ranges of these parameters for purposes of instrumentation applicability, we have relied on experimental observations where reported. In many cases, such information is not available. In these cases, we have made our best estimate based on related media information and/or expert opinion.

2.0 CRITICAL PARAMETERS FOR TUFF

In developing the lists of critical parameters for tuff, consideration was given to the relative importance of those parameters in specific discipline areas: geomechanics, geology, hydrology, and geochemistry. The relative importance of the parameters was considered for each phase of repository activity: site characterization, site construction, site operation (including retrievability), and site closure and decommissioning.

The time frames of interest for the different parameters are illustrated in Fig. 1. This chart, which contains both instrumented and noninstrumented parameters, follows the need to measure a specified parameter through the repository phases under consideration. Though federal regulations do not presently require measurements after repository closure, it seems prudent to assume that it will be highly likely that certain measurements will continue to be made. These measurements are listed under the "Closure and Decommissioning Phase" of Fig. 1 and in Tables 4 and 8. However, we assume that no measurements will be made that require physical penetration into the repository after closure. Future instrumentation technology may allow continued *in situ* repository monitoring using as yet undefined remote sensing or isolated communications techniques.

Site characterization, construction, operation, and closure and decommissioning are not necessarily distinct time periods, but may overlap each other. For example, site characterization activities may continue completely through the construction phase of the repository, and operation may start in one underground location well before the total completion of construction in another location of the same repository.

Based on the time-line considerations and on the parameter requirements in each discipline area, composite listings of the parameter needs for each repository phase were developed. The authors, who have expertise in each of these discipline areas, singly or as a group, considered the relative importance of parameters on a qualitative scale for each repository phase in tuff. The relative rankings of these parameters for general tuff are shown in Tables 1 through 4. The relative ranking of parameters within any single numerically designated priority level in these tables is not necessarily listed in any subpriority

Parameter and Discipline[a]	Repository Phase and Priority Level[b]			
	Site Characterization	Construction	Operations (Including Retrievability)	Closure and Decommissioning
Hydrostratigraphic unit depth, thickness, orientation and continuity* (H)	(1)	(4)		
Water infiltration rate (H)	(1)	(4)	(5)	(2)
Groundwater recharge and discharge locations and rates (H)	(1)	(4)	(5)	(2)
Permeability (fracture and matrix) (H)	(1)	(4)		
Water saturation (H)	(1)	(1)	(1)	(2)
Water potential (H)	(1)	(1)	(2)	(2)
Saturation characteristics (pressure head *vs* saturation) (H)	(1)			
Relative permeability (water and air) (H)	(1)			
Fluid velocity (H)	(1)		(2)	(2)
Porosity and distribution of pore sizes (H)	(1)	(4)		
Age of water (C)	(1)	(1)		
Geologic variables (lithologic parameters, etc.)** (G)	(1)	(2)	(3)	
Sorptive capacity of formation rock (C)	(1)			
Thermal conductivity, heat capacity, and diffusivity (M)	(1)			
Convective heat transfer (M)	(1)		(1)	
Temperature (M)	(1)	(4)	(1)	(2)
Fracture properties (aperture) (M)	(2)	(1)		
Fracture properties (spacing, orientation, continuity, and connectivity)* (M)	(2)	(1)		
Groundwater chemistry (C)	(3)	(3)	(3)	
Solubility of radionuclides of interest (C)	(3)			
Volatility and gaseous diffusion of radionuclide chemical species (C)	(3)			
Canister and support system corrosion (C)	(3)		(4)	(1)
Initial *in situ* stress (M)	(3)	(2)		
In situ stress changes (M)	(3)	(1)	(3)	
Displacement and deformation (M)	(3)	(1)	(2)	
Rock modulus and Poisson's ratio (M)	(3)	(2)	(3)	
Expansivity (M)	(3)			
Rock strength (M)	(3)	(1)		
Induced fractures (M)	(3)	(1)	(1)	
Water inflow rate (H)	(4)	(3)	(5)	
Tectonic factors (faulting and folding)** (G)	(4)	(2)		
Tectonic factors (seismicity) (G)	(4)	(2)	(5)	(3)
Potential igneous activity* (G)	(4)			
Seal and backfill properties (H)	(5)		(4)	(1)
Seal and backfill leakage (C)	(5)		(4)	(1)
Decrepitation and spalling (M)	(5)		(4)	
Crustal deformation, including uplift (G)	(6)	(5)	(5)	(3)
Erosion rate** (G)	(6)	(5)	(6)	(3)
Naturally occurring radionuclides (G)	(6)			
Water, mineral, and petroleum resources* (G)	(7)			
Radionuclide leakage rate (C)			(4)	(1)
Canister movement (M)			(5)	

(a) Disciplines are given by: (M)=Geomechanics, (G)=Geology, (H)=Hydrology, (C)=Geochemistry.

(b) Parameter priority levels are given in parentheses for each repository phase, (1) being highest priority.

* Not dependent on instrumentation.

** Not directly dependent on instrumentation, but may use some geophysical techniques.

Figure 1. Critical parameter time line for a repository in tuff.

Table 1. Prioritized critical parameters for site characterization, tuff.

Priority level	Critical parameters
1.	Hydrostratigraphic unit depth, thickness, orientation, and continuity
	Hydrologic parameters - water infiltration rate - groundwater recharge and discharge locations and rates - permeability (fracture and matrix) - water saturation - water potential - saturation characteristics (pressure head *vs* saturation) - relative permeability (water and air) - fluid velocity - porosity and distribution of pore sizes
	Age of water
	Geologic variables, lateral and vertical variations in - lithology (including lithophysal zones) - mineralogy - stratigraphy - bedding
	Sorptive capacity of formation rock
	Thermal properties - thermal conductivity - heat capacity - thermal diffusivity
	Convective heat transfer
	Temperature
2.	Fracture properties - spacing - orientation - aperture - continuity - connectivity
3.	Groundwater chemistry - composition - pH - Eh
	Solubility of radionuclides of interest
	Volatility and gaseous diffusion of radionuclide chemical species
	Canister and support system corrosion (tests) - steam fraction, gas content, and temperature at canister surface
	Initial *in situ* stress
	In situ stress changes
	Displacement and deformation
	Rock modulus and Poisson's ratio
	Expansivity
	Rock strength
	Induced fractures (and excavation damage)
4.	Water inflow rate
	Tectonic factors - faulting - folding - seismicity
	Potential igneous activity
5.	Seal and backfill properties (tests)
	Seal and backfill leakage (tests)
	Decrepitation and spalling (tests)
6.	Crustal deformation, including uplift
	Erosion rate
	Naturally occurring radionuclides
7.	Water, mineral, and petroleum resources

Table 2. Prioritized critical parameters for site construction, tuff.

Priority level	Critical parameters
1.	Fracture properties - spacing - orientation - aperture - continuity - connectivity
	Induced fractures (and excavation damage)
	Hydrologic parameters - water saturation - water potential
	Age of water
	Displacement and deformation
	In situ stress changes
	Rock strength
2.	Initial *in situ* stress
	Rock modulus and Poisson's ratio
	Tectonic factors - faulting - folding - seismicity
	Geologic variables, lateral and vertical variations in - lithology (including lithophysal zones) - mineralogy - stratigraphy - bedding
3.	Groundwater chemistry - composition - pH - Eh
	Water inflow rate
4.	Hydrostratigraphic unit depth, thickness, orientation, and continuity
	Hydrologic parameters - Permeability (fracture and matrix) - Porosity and distribution of pore sizes - Groundwater recharge and discharge locations and rates - Water infiltration rate
	Temperature
5.	Crustal deformation, including uplift
	Erosion rate

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Table 3. Prioritized critical parameters for site operation, tuff.

Priority level	Critical parameters
1.	Temperature Convective heat transfer Water saturation Induced fractures
2.	Water potential Fluid velocity Displacement and deformation
3.	Groundwater chemistry - composition - pH - Eh *In situ* stress changes Rock modulus and Poisson's ratio Geologic variables (changes in mineralogy due to heating)
4.	Canister and support system corrosion - steam fraction, gas content, and temperature at canister surface Seal and backfill properties Seal and backfill leakage Radionuclide leakage rate Decrepitation and spalling
5.	Tectonic factors - seismicity Crustal deformation, including uplift Groundwater recharge and discharge locations and rates (changes) Water inflow rate Water infiltration rate Canister movement
6.	Erosion rate

Table 4. Prioritized critical parameters for site closure, tuff.

Priority level	Critical parameters
1.	Radionuclide leakage rate
	Seal and backfill leakage
	Seal and backfill properties
	Canister corrosion rate (simulated in test facility) - steam fraction, gas content, and temperature at canister surface
2.	Hydrologic parameters - water infiltration rate - groundwater recharge and discharge locations and rates (changes) - fluid velocity - water potential - water saturation
	Temperature
3.	Tectonic factors - seismicity
	Crustal deformation, including uplift
	Erosion rate

order. Within numerically designated levels, parameters are considered to have equal priority.

It should be noted that the relative ranking of closely spaced (in importance) parameters is only approximate and could change significantly, depending on site-specific considerations and increased understanding of parameter importance. In addition, a different group of experts may develop a slightly different relative ranking, and these factors are recognized. However, the relative importance of parameters near the top of each table will likely continue to be greater than those near the bottom of each table, irrespective of site-specific considerations or different expert interpretation.

In terms of the analysis of the different measurement techniques and instruments for the listed parameters, it is useful to separate the parameters listed in Tables 1 through 4 into specific disciplines (*i.e.*, geomechanical, geological, hydrological, and geochemical). In addition, Tables 1 through 4 contain both instrumented and noninstrumented parameters. We have included the noninstrumented parameters for completeness because these need to be known to establish repository adequacy. In Tables 5 through 8 the critical parameters are listed by repository phase and discipline area, and a differentiation is made between the instrumented and noninstrumented parameters. Within a given phase and discipline area, the relative parameter importance is rank ordered, however, this rank ordering is subject to the caveats discussed in the preceding paragraph and should be used only for general guidance. Considerations which may affect the relative parameter importance within a given discipline area or repository phase are discussed in Section 3.0 on Detailed Critical Parameter Considerations.

Table 5. Prioritized critical parameters by discipline for site characterization, tuff.

GEOMECHANICAL PARAMETERS

Instrumented

- Thermal properties
  - thermal conductivity
  - heat capacity
  - thermal diffusivity
- Convective heat transfer
- Temperature
- Fracture properties
  - aperture
- Initial *in situ* stress
- *In situ* stress changes
- Displacement and deformation
- Rock modulus and Poisson's ratio
- Expansivity
- Rock strength
- Induced fractures (and excavation damage)
- Decrepitation and spalling (tests)

Noninstrumented

- Fracture properties
  - spacing
  - orientation
  - continuity
  - connectivity

GEOLOGIC PARAMETERS

Instrumented

- Tectonic factors
  - seismicity
- Crustal deformation, including uplift
- Naturally occurring radionuclides

Noninstrumented

- Geologic variables, lateral and vertical variations in
  - lithology (including lithophysal zones)
  - mineralogy
  - stratigraphy
  - bedding
- Tectonic factors
  - faulting
  - folding
- Potential igneous activity
- Erosion rate
- Water, mineral, and petroleum resources

HYDROLOGIC PARAMETERS

Instrumented

- Water infiltration rate
- Groundwater recharge and discharge locations and rates
- Permeability (fracture and matrix)
- Water saturation
- Water Potential
- Saturation characteristics (pressure head *vs* saturation)
- Relative permeability (water and air)
- Fluid velocity
- Porosity and distribution of pore sizes
- Water inflow rate
- Seal and backfill properties (tests)

Noninstrumented

- Hydrostratigraphic unit depth, thickness, orientation, and continuity

GEOCHEMICAL PARAMETERS

Instrumented

- Age of water
- Sorptive capacity of formation rock
- Groundwater chemistry
  - composition
  - pH
  - Eh
- Solubility of radionuclides of interest
- Volatility and gaseous diffusion of radionuclide chemical species
- Canister and support system corrosion (tests)
  - steam fraction, gas content, and temperature at canister surface
- Seal and backfill leakage (tests)

9

Table 6. Prioritized critical parameters by discipline for site construction, tuff.

GEOMECHANICAL PARAMETERS	GEOLOGIC PARAMETERS	HYDROLOGIC PARAMETERS	GEOCHEMICAL PARAMETERS
Instrumented Fracture properties - aperture Induced fractures (and excavation damage) Displacement and deformation *In situ* stress changes Rock strength Initial *in situ* stress Rock modulus and Poisson's ratio Temperature	**Instrumented** Tectonic factors - seismicity Crustal deformation, including uplift	**Instrumented** Water saturation Water potential Water inflow rate Permeability (fracture and matrix) Porosity and distribution of pore sizes Groundwater recharge and discharge locations and rates Water infiltration rate	**Instrumented** Age of water Groundwater chemistry - composition - pH - Eh
Noninstrumented Fracture properties - spacing - orientation - continuity - connectivity	**Noninstrumented** Tectonic factors - faulting - folding Geologic variables, lateral and vertical variations in - lithology (including lithophysal zones) - mineralogy - stratigraphy - bedding Erosion rate	**Noninstrumented** Hydrostratigraphic unit depth, thickness, orientation, and continuity	

Table 7. Prioritized critical parameters by discipline for site operation, tuff.

GEOMECHANICAL PARAMETERS	GEOLOGIC PARAMETERS	HYDROLOGIC PARAMETERS	GEOCHEMICAL PARAMETERS
Instrumented	**Instrumented**	**Instrumented**	**Instrumented**
Temperature Convective heat transfer Induced fractures Displacement and deformation *In situ* stress changes Rock modulus and Poisson's ratio Decrepitation and spalling Canister movement	Tectonic factors - seismicity Crustal deformation, including uplift **Noninstrumented** Geologic variables (changes in mineralogy due to heating) Erosion rate	Water saturation Water potential Fluid velocity Seal and backfill properties Groundwater recharge and discharge locations and rates (changes) Water inflow rate Water infiltration rate	Groundwater chemistry - composition - pH - Eh Canister and support system corrosion - steam fraction, gas content, and temperature at canister surface Seal and backfill leakage Radionuclide leakage rate

Table 8. Prioritized critical parameters by discipline for site closure, tuff.

GEOMECHANICAL PARAMETERS	GEOLOGIC PARAMETERS	HYDROLOGIC PARAMETERS	GEOCHEMICAL PARAMETERS
Instrumented Temperature	**Instrumented** Tectonic factors - seismicity Crustal deformation, including uplift **Noninstrumented** Erosion rate	**Instrumented** Seal and backfill properties Water infiltration rate Groundwater recharge and discharge locations and rates (changes) Fluid velocity Water potential Water saturation	**Instrumented** Radionuclide leakage rate Seal and backfill leakage Canister corrosion rate (simulated in test facility) - steam fraction, gas content, and temperature at canister surface

3.0 DETAILED CRITICAL PARAMETER CONSIDERATIONS

Consideration of the adequacy of a measurement technique or instrument for a given parameter or group of parameters depends on detailed knowledge of the measurement problems and environment, the parameter range of interest, and the accuracy with which the parameter must be determined. Such considerations are obviously medium and site specific. In considering the parameters identified in Section 2.0, the parameter's role during each repository phase and its interaction with other parameters are addressed where appropriate. A number of other questions and factors are also considered as follows:

1. Normal Parameter Range
2. Is this parameter site sensitive?
3. Expected parameter variations during normal site operation.
4. Parameter values that may signal trouble (where sufficient information is available).
5. What may happen if this parameter is not measured?
6. Measurement conditions and potential instrumentation problems.

While each consideration indicated above may not apply to each parameter, they were considered useful and were used as guides in the following discussions. Due to the relative variations in parameter priorities between the different repository phases, no attempt was made to discuss each parameter in priority order. Rather, the parameter and specific consideration regarding that parameter are treated by discipline. Due to the extensive data base acquired from experiments in tuffaceous rock at the Nevada Test Site (NTS), specific examples of parameters measured or extrapolated from that work are used for discussion where appropriate. Note that closely related parameters are discussed jointly due to their interdependence or similarity.

3.1 Geomechanical Parameters

Geomechanical parameters discussed in the following sections include those parameters that directly interrelate stresses, physical responses, thermal characteristics, and thermomechanical properties within the repository media. Except for cataloging certain fracture characteristics, all are considered to be parameters generally requiring instrumentation for measurement or monitoring.

3.1.1 Displacement and Deformation

The rock mass around a repository will deform as a result of disturbances caused by construction and waste emplacement. Displacement and deformation measurements will be performed during the site characterization phase as part of *in situ* tests where constitutive laws for the rock mass will be quantified. Data from measurements during site characterization will also be used to help validate predictive models to be used for repository design and performance evaluation. Displacement and deformation measurements will be performed to monitor rock behavior during the construction and operation phases to verify the adequacy of the repository design, to confirm the validity of predictive models used, and to monitor the stability of the repository.

Rock displacement and deformation are closely related to rock stability and to the capability to retrieve the waste. Excessive rock displacement or deformation may affect the waste package. They may also affect the movement of water, steam, and gas through the rock by causing the opening or closing of fractures. The rock deformations measured around a repository will be a complex function of the *in situ* mechanical and thermomechanical properties of the rock mass and its discontinuities, the state of stress, and the temperature of the rock.

In fractured tuff, most of the measured displacement will occur along fractures because they are the most deformable elements of the rock mass system. Consequently, measured displacements are related to various fracture characteristics (*e.g.*, orientation, roughness and waviness, fracture frequency, filling minerals and their moisture contents). The measured displacements and deformations will also be a function of the orientation of the underground workings relative to the major principal stress axes.

It is clear from the preceding paragraphs that rock displacement and deformation interact

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with many of the other critical parameters. Displacements along fractures, and deformations that influence changes in fracture apertures will influence fracture permeabilities. This can, in turn, influence fluid velocities within the rock and water inflow rates into the repository, though water inflow may not be a serious problem in the unsaturated region. Displacement and deformation will be directly influenced by the state of initial *in situ* stress in the rock, rock elastic modulus and Poisson's ratio, rock strength, the coefficient of thermal expansion, and creep characteristics. However, plastic deformation, or creep, is not considered a critical parameter in tuff. Geologic variables such as lithophysal cavities, open or filled, will also influence rock mass deformations.

The displacements and deformations will result in *in situ* stress changes, and manifest themselves in induced fractures, decrepitation and spalling, crustal deformation, and changes in seal and backfill permeabilities, which can affect radionuclide leakage through the seals and backfill. The interaction between displacement and deformation and fracture properties has already been discussed.

Thermal expansion will be one of the principal driving forces of rock deformations, stress changes, and, consequently, displacements within a repository in tuff. The thermal expansion (which includes thermal contraction) is directly influenced by changes in the temperature field, which are influenced by the thermal conductivity and heat capacity of the rock mass. Thermal diffusivity is completely defined by thermal conductivity and heat capacity. Hydraulic flow and convective heat transfer, including such effects as heat piping (which can easily occur in an unsaturated medium), will also influence temperature distribution within the rock, and, hence, displacement and deformation. Displacement and deformation will complete the circle with their influence on convective heat transfer and hydraulic flow.

3.1.1.1 Normal parameter range

Deformations resulting from stress changes during repository construction and from thermal expansion of the rock following waste emplacement are expected to be in the order of millimeters over the distance of a few meters (Zimmerman *et al.*, 1984; Tillerson and Nimick, 1984; Zimmerman *et al.*, 1985). Normal deformation in unconfined welded tuff is approximately 1 mm/m for an average temperature change of 100°C (DOE, 1984, Section 6.3.1.3). However, for the purpose of *in situ* deformation measurements, much of the driving force from thermal expansion will result in stress changes within the rock and closure of fractures and lithophysal cavities rather than in substantial deformations integrated by measurements over a distance of several meters. On the other hand, displacements resulting from rock failure or shear along fracture planes can be considerably larger than confined deformations. For that reason instruments used to measure deformations and displacements over distances of several meters (or a few tens of meters) should have the range to accommodate displacements of several centimeters and yet have the resolution to adequately measure small increments of deformation and displacement down to at least 0.1 mm (or preferably to 0.01 mm, especially during site characterization tests and experiments).

3.1.1.2 Are these parameters site sensitive?

Deformations and displacements are directly related to the *in situ* mechanical properties of the rock mass and lithologic variables, which are site sensitive. Thus, these parameters are also site sensitive.

3.1.1.3 Expected parameter variations during normal site operation

Displacements and deformations will be complex functions of multiple variables. Thus, the expected parameter variations are difficult to predict precisely with the limited information presently available.

3.1.1.4 Parameter values that may signal trouble

In the long-term, accelerating displacement or deformation rates occurring after periods of relatively constant changes will be indicative of areas of potential instability. Displacements and deformations greater than the normal parameter range may be indicative of mechanical instability. In addition, even small changes can change the permeability of the rock, hence, causing changes in the capillary characteristics of the rock that influence the movement of liquid-phase water in the unsaturated region. Gas phase (water vapor) movement through the rock can be dramatically affected by changes in permeability (see Sections 3.3.2 and 3.3.3, Permeability, and Relative Permeability).

3.1.1.5 What may happen if these parameters are not measured?

Absolute displacements and deformations and their rates are two very important diagnostic responses of rock behavior. In concept, these parameters are easy to measure *in situ* and with proper attention can be measured accurately and reliably. Displacement and deformation measurements spanning several meters integrate the effects of inhomogeneous mechanical properties in the rock. Without measurements of deformation, constitutive laws relating stress and strain cannot be quantified; thus, models used to predict repository behavior cannot be validated.

Verification of the repository design cannot be performed without displacement and deformation measurements. Potential areas of instability will not be adequately monitored because excessive displacements or deformations indicative of unstable rock zones will not be adequately monitored.

Rock deformation can be back calculated from measurements of stress changes and of modulus of deformation. This approach is not commonly used because it may provide unreliable results in rock masses which are substantially inelastic (*e.g.*, highly fractured tuff).

3.1.1.6 Measurement conditions and potential problems

Displacements and deformations measured in tuff will probably occur along fractures and into lithophysae because they tend to be the most deformable elements in the rock mass. Consequently, measurements of displacements and deformations are likely to vary throughout the area of the repository because of the variable nature of the fracture network and lithophysae. Relatively large displacements may be measured in volumes of the rock with larger fracture densities. It may also be difficult to anchor measurement instruments in fractured and lithophysal regions of rock. Instruments to measure deformations over distances of a few centimeters, and anchors for instruments that are used to measure deformations over longer distances or across fractures and voids, must be emplaced in intact and relatively homogeneous rock.

3.1.2 Fracture Properties and Induced Fractures

The Topopah Springs Member of the Paintbrush Tuff contains the horizon being considered as the potential host rock for a repository. This horizon is located in a thickly welded devitrified zone containing abundant lithophysae in several intervals, but they are most common in the upper and central portions. The lithophysae is less abundant in the lower part of the densely welded interval preferred as the host rock for the repository. However, the densely welded portions of the Paintbrush Tuff are more intensely fractured than other portions (DOE, 1984, Section 3.2.1.3).

Rock displacement and deformation, mechanical strength and stability, and groundwater movement will be strongly influenced by fracture networks in the tuff. Fracture permeability in the unsaturated tuff surrounding the preferred horizon will affect fluid velocities through the tuff, water inflow rates into repository openings, and convective heat transfer. Capillary pressures controlling liquid-phase water movement in the unsaturated tuff will be influenced by fracture and matrix permeabilities. Closure of large fractures that act as capillary barriers when open can have a strong effect on both liquid- and gas-phase water flow paths.

New fractures may be induced by repository construction or radiogenic heating from emplaced waste. Thermal degradation in the forms of decrepitation and spalling may occur in the hottest zones of rock. Rock bursts (sudden release of strain energy related to high-stress concentrations around openings) can cause new fractures, and massive (unfractured) rock may be susceptible to fracturing, if surrounded by deformable rock, as a result of stress concentration that may develop in the massive rock.

Various fracture characteristics affect rock behavior. Important among these are: the abundance of fractures (absolute spacing, fracture density), their geometrical and statistical characteristics (orientation, length, aperture), surface roughness and waviness, and connectivity of fractures.

A number of important rock properties and parameters are affected by the presence of fractures in the rock mass. Rock deformation and rock modulus of deformation are affected by fracture roughness, orientation, persistence, spacing, and aperture, as well as by the character of filling materials. Rock mass strength is influenced by water distributions within the fractures. Rock permeability is governed by fracture density, aperture, filling materials, continuity, and connectivity. The state of stress around underground openings can also be affected by fractures; and fracturing, in turn, can be influenced by the state of stress.

From the preceding discussions it is apparent that fracture properties and induced fractures can interact significantly with the following other critical parameters:

- fracture permeability
- relative permeabilities (water and air)
- fluid velocity
- water inflow rate
- radionuclide leakage
- rock strength
- displacement and deformation
- rock modulus and Poisson's ratio
- initial *in situ* stress
- *in situ* stress changes
- convective heat transfer
- temperature
- expansivity
- decrepitation and spalling

In a repository scenario, characterization investigations should be sufficiently detailed to detect the fractures that control the mechanical and hydrologic response of the rock mass. The anisotropy and inhomogeneity of various rock properties are also greatly influenced by fracture systems. During the site characterization phase, fracture properties such as spacing, orientation, continuity, and connectivity must be characterized along with other properties that influence rock strength. The influence of changes in stress fields on fracture apertures must be measured. Fracture mapping, characterization, and measurements to monitor aperture changes should move into the new rock as openings are mined during the site construction phase.

Measurements to detect and characterize induced fracturing and excavation damage should be made during the construction of underground test facilities for site characterization. They also will be an integral part of the site characterization experiments and tests involving thermal and mechanical loading of the rock. Monitoring to detect and locate induced fracturing as a result of excavation should continue during repository construction. Measurements should also continue during the site operations phase to detect and locate induced fracturing caused by thermal loading from the waste canisters.

3.1.2.1 Normal parameter range

The Topopah Springs Member of the Paintbrush Tuff is considered to be highly fractured. However, many of the fracture attributes, such as orientation, frequency, length, and aperture, have not been measured. Virtually no data are available on properties of individual fractures or the effect of fractures on rock matrix properties (DOE, 1984, Section 6.3.1.3). Fracture characteristics are expected to be similar to those encountered in the welded tuff of G-tunnel with fracture spacings of 1 m or less (Tillerson and Nimick, 1984).

3.1.2.2 Are these parameters site sensitive?

Fractures are, by nature, spatially variable even within a given rock unit. Consequently, all fracture characteristics are highly site specific.

3.1.2.3 Expected parameter variations during normal site operation

Fracture aperture will change as the rock mass deforms in response to the repository environment. This can significantly influence hydrologic parameters. The composition and water content of minerals filling the fractures will also change as rock temperature changes. For canister heat loads of 3.3 kW/canister, thermomechanical calculations predict a potential for rock fracturing in the immediate vicinity of the waste-emplacement hole, extending less than 10 cm into the rock (DOE, 1984, Section 6.3.1.3.4).

3.1.2.4 Parameter values that may signal trouble

Of particular concern are any near-vertical fractures which may connect the repository horizon to saturated regions below it. Steeply dipping fractures trending parallel, or at an acute angle, to repository openings can cause roof instability. Unstable rock may exist in areas where spacing between fractures is smaller than the width of the tunnel rooms and where these fractures combine to form unstable blocks or wedges. Near horizontal fractures may also affect roof stability depending on fracture spacing, continuity, orientation with respect to stress directions, and proximity to stress concentrations. Acoustic emission and microseismic remote-sensing techniques should be used to monitor for induced fracturing and potential rock burst conditions.

3.1.2.5 What may happen if these parameters are not measured?

Repository performance can only be predicted with a low level of confidence if fracture characteristics are not known. Results of *in* *situ* tests designed to investigate the mechanical and hydrological properties of rocks cannot be correctly interpreted without fracture measurements, because fractures will affect these results. Areas of potential instability are unlikely to be adequately monitored because they will be unidentifiable without fracture information. Radionuclides may escape unpredictably through fracture flow paths which have not been detected. New fractures caused by the construction or operation of the repository can cause new flow paths which will change the hydrological response of the rock mass. Unexpected releases of radionuclides may occur and their magnitude, discharge locations, and flow rates will be unknown if the characteristics of these fractures are unknown.

Without adequate information on fracture characteristics, retrievability cannot be guaranteed because failure of the underground workings, including rock burst, could occur unpredictably. Fracture information is required to properly place instruments that will monitor rock behavior. Excessive deformation, occurring along fractures, and induced fracturing, can affect the integrity of waste packages and the waste form.

3.1.2.6 Measurement conditions and potential instrumentation problems

The characteristics of the fracture network are likely to vary both laterally and vertically. Fracture orientation and density, for example, should be expected to be spatially variable. Such instruments as borehole stress meters, borehole deformation gauges, and extensometer anchors should be located in intact rock sections (*i.e.*, not at fractures), or their effectiveness can be questionable in an intensely fractured medium such as the Topopah Springs welded tuff.

Of critical importance are those fractures which interconnect with other fractures to create lateral or vertical flow paths connecting the repository horizon with other permeable units. Since it is necessary to minimize the number of penetrations between repository drifts and the underlying water table, fracture mapping using vertically inclined borehole cores will also be held to a minimum. It is important, therefore, to further develop remote sensing and indirect methods to characterize rock properties from repository drifts. Such methods can include seismic, microseismic, and ultrasonic techniques, acoustic emission measurements, as well as electrical and electromagnetic measurement techniques. Hydrologic tests can also provide valuable fracture information.

3.1.3 Initial *In Situ* Stress and Stress Changes

The rock mass surrounding an HLW repository will contain stress components due to the weight of overlying materials, confinement, and tectonic processes. The initial stress state of the rock will be disturbed by repository construction and by thermal loading from the emplaced waste. Consequently, the virgin state of stress in the rock and stress changes due to repository construction and operation are of concern. The magnitude and orientation of stresses around underground workings are directly related to rock behavior, and need to be known to predict stability and deformation of structures in the rock. Knowledge of initial stresses is necessary to properly design subsurface repository workings, and stress changes also affect the stability and deformations of the repository tunnels and emplacement boreholes.

During the site characterization phase, measurements of initial stresses will provide baseline information with which to assess potential for rock failure and rock bursts, and provide information needed to properly design and construct the underground repository facilities. Measurements of stress changes performed during *in situ* tests will help to provide an understanding of the physical response of the rock to various phenomena, and provide information required to quantify constitutive laws which describe rock mass response to thermal, hydraulic, and mechanical perturbations.

After the site characterization phase, measurements of stress changes, used in conjunction with measurements of displacement and deformation, will serve to monitor rock mass behavior. These measurements are also needed to validate models and verify the adequacy of the repository design. Measurements of initial stresses should be performed during construction in any newly excavated areas where a different state of stress is suspected as a result of differences in geologic conditions. Continuous measurements of stress changes should be made during the site construction and operation phases to monitor the effects of repository construction and thermal loading.

The usefulness of stress measurements is directly related to the confidence with which they can be used. Stress information is meaningless unless it is used in conjunction with other geotechnical parameters, such as rock mass strength and rock modulus of deformation. Therefore, the accuracy with which rock mass strength and modulus of deformation are measured will partially control the usefulness of stress measurements. The relative importance of stress measurements is roughly equal to that of rock mass strength and modulus of deformation measurements.

The state of stress not only affects the geomechanical behavior of a rock mass, but also the movement of groundwater. Stresses cause fractures to deform and change their aperture. Thus, the permeability of fractures to steam, water, and air can change with changes in stress. In the unsaturated tuff this could result in significant variations in convective heat transfer following waste emplacement.

The state of stress in the host rock of a repository will be a complex function of several variables: the depth of the repository, regional stresses, geologic structures and discontinuities, variations in surface or basement rock topography, thermal loading, and the underground openings present. The state of stress will also be a function of the *in situ* mechanical properties of the rock mass. A spatially variable state of stress can be expected in tuff because *in situ* mechanical properties are likely to be inhomogeneous, especially in zones containing abundant lithophysae.

The state of stress or changes in the state can be back-calculated from measurements of deformation (or strain), if accurate moduli of rock deformation are used. Geophysical parameters, such as the propagation velocity of seismic waves, cross-hole ultrasonics, and acoustic emission, may prove to be reliable indicators of changes of stress (Paulsson *et al.*, 1980; Paulsson, 1983).

3.1.3.1 Normal parameter range

At the depths in which the repositories will be constructed, a reasonable assumption is that the vertical normal stress is directly proportional to the weight of the overburden. The ratio of horizontal *in situ* stress to vertical *in situ* stress in welded and non-welded tuff of the G-Tunnel complex falls in the range of 0.5 to 1.0 (Johnstone *et al.*, 1984). The average and limit vertical stresses and ratios of horizontal stress to vertical stress are given in Table 9 for four stratigraphic units of the Yucca Mountain tuff at potential repository horizon depths.

Table 9. Near-field *in situ* stresses in Yucca Mountain tuffs (Johnstone *et al.*, 1984).

	Topopah Springs	Calico Hills	Bullfrog	Tram
Average				
σ_v [MPa]	8.6	10.3	16.8	20
σ_h/σ_v	0.96	0.87	0.72	0.70
Limit				
σ_v [MPa]	11.3	15.4	20.6	23.7
σ_h/σ_v	0.96	0.87	0.72	0.70

3.1.3.2 Are these parameters site sensitive?

Many of the factors affecting the state of stress are geological conditions which are site specific (*e.g.*, regional stresses, fracture characteristics). Thus, measurements of the initial state of stress will be site specific. Changes in stress, caused by man's activities, will also be site specific because they are controlled by the inhomogeneity of the mechanical properties within the tuff.

3.1.3.3 Expected parameter variations during normal site operation

Quantitative values are not known at present. However, stress changes will be created by repository excavation and thermal loading. The Topopah Springs Member is already highly fractured, and it is therefore expected that significant thermally induced expansion can occur without generating sufficient stresses to cause new fracturing (DOE, 1984, Section 6.3.1.3.3). This assumption should be tested during site characterization experiments.

3.1.3.4 Parameter values that may signal trouble

At repository depths, initial stresses can be high enough to trigger rock failure. Changes in the initial state of stress caused by construction and waste emplacement can also cause rock instability and failure. Goodman (1980) indicates that rock failure can be expected to occur whenever the major principal stress is more than about 25% of the unconfined compressive strength of the rock.

3.1.3.5 What may happen if these parameters are not measured?

Initial stresses must be known to adequately design a repository and to evaluate its short-term stability. Inadequate repository design may result in excessive deformation of emplacement tunnels and boreholes, damage to waste packages, or instability of roofs and walls of the excavations. Changes in stress created during *in situ* testing are needed to establish the physical response of rock to various phenomena. Stress measurements are also used to quantify the constitutive laws that predict rock behavior. If stress changes are not monitored during *in situ* tests, the constitutive laws needed to predict repository behavior cannot be quantified. Furthermore, predictive model validation and repository design verification cannot be accomplished without state of stress information. Knowledge of *in situ* stress and stress changes is important during the site construction and operations phases because of their influence on induced fracturing and potential rock burst.

3.1.3.6 Measurement conditions and potential instrumentation problems

The state of stress in a tuffaceous rock mass will vary because *in situ* mechanical properties of tuff are variable. Consequently, measurements of stress should be made at numerous locations throughout the repository to adequately characterize the stress field. However, even precise stress measurements obtained in an inhomogeneous geologic environment will be difficult to relate directly to repository performance. Considerable judgment will be required to interpret and apply the results.

3.1.4 Rock Strength

Rock strength parameters describe the failure behavior of rock (where failure is defined as that load at which the rock ceases to perform satisfactorily). Important rock strength parameters needed for repository design and safety analysis include compressive strength, matrix (intact rock) tensile strength, and matrix cohesion and angle of internal friction; and such fracture properties as cohesion and coefficient of friction. In the highly fractured welded tuff of the Topopah Springs Member, the shear strength of fractures will likely control the overall strength of the rock mass. Fracture shear strength is described by the peak and residual angles of joint friction, the cohesion, and the stiffness of the joint. Extensive characterization of rock strength properties must be done during the site characterization phase under test conditions that include variations in temperature, water content, and confining stress. Rock strength tests must continue during site construction into newly excavated rock where rock strength properties may vary due to differences in geologic conditions.

Rock strength parameters are used in conjunction with state of stress information to design the repository and to predict the stability of the rock mass. Rock strength varies with rock porosity, temperature, and confining stress. Various fracture characteristics strongly affect rock strength (*i.e.*, fracture density; fracture roughness and waviness; fracture orientation, continuity and connectivity; and fracture filling materials, and their moisture content). The shear strength of fractures is related to the displacements which occur along the fracture plane, because roughness of the fracture surfaces can cause joint dilatancy during displacement. This phenomenon alters the state of stress acting on the fractures and their resistance to failure. Because rock strength can affect fracture apertures, it can also influence fracture permeability and relative permeability (to steam, water, and air), fluid velocities and water inflow rates, and convective heat transfer. Rock strength properties also influence the susceptibility of rock to induced fracturing, and decrepitation and spalling; and, conversely, these parameters influence rock strength.

Because fracture characteristics are spatially variable and anisotropic, rock strength parameters are also spatially variable and anisotropic. This is particularly true when comparing zones of welded and unwelded tuff, and where there are large variations in lithophysal content when considering the integrated strength of larger rock masses.

3.1.4.1 Normal parameter range

A limited number of rock strength property measurements have been made on Yucca Mountain tuff in four potential repository horizons. Table 10 summerizes the rock strength parameter measurements for the most likely candidate horizon, which is located in the Topopah Springs Member of the Paintbrush Tuff. The Topopah Springs data are for welded tuff assumed to contain 5% lithophysae. Preliminary tests indicate

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Table 10. Summary of rock strength parameters for Topopah Springs Member tuff (Tillerson and Nimick, 1984; Johnstone *et al.*, 1984).

Parameter	Value
Unconfined compressive strength	95.9 ± 35.0 MPa
Matrix cohesion	28.5 MPa
Angle of internal friction	26.0°
Matrix tensile strength	12.8 ± 3.5 MPa
Joint cohesion	1 MPa
Coefficient of friction for initiation of joint sliding	0.8

that compressive strength decreases with increased porosity and/or increased water content. The dependence of rock strength properties on water content, confining stress, and temperature is still under investigation (DOE, 1984, Section 6.3.1.3.2).

The current data for Topopah Springs matrix rock shows essentially elastic behavior up to the onset of brittle failure (DOE, 1984, Section 6.3.1.3.3). Though the Topopah Springs tuff is highly fractured, the rock mass is expected to be strong, with little likelihood that blocks will fall on waste canisters and breach containment, although experience and *in situ* testing will be needed to confirm this (DOE, 1984, Section 6.3.1.3.3). It is also expected that access drifts and underground openings can be supported by conventional rockbolts, wire mesh, and shotcrete (DOE, 1984, Section 5.2.1).

3.1.4.2 Is this parameter site specific?

The stratigraphic section at Yucca Mountain is composed of a sequence of welded and nonwelded tuffs; some strata are devitrified or altered, and some remain vitric (DOE, 1984, Section 6.3.1.3.2). There is also considerable variation in lithophysal content at various depths within any one particular stratigraphic unit. These inhomogeneities, along with the strong influence of fractures on rock strength parameters and the inhomogeneous nature of fracture systems, make rock strength parameters very site specific.

3.1.4.3 Expected parameter variations during normal site operation

The dependence of rock strength properties on water content, confining stress, temperature, and time have not yet been determined.

3.1.4.4 Parameter values that may signal trouble

Goodman (1980) has stated that whenever the major stress in a region is more than about 25% of the unconfined compressive strength of the rock, rock failure can be expected. This "rule of thumb" is useful as an estimate of instability if the rock is relatively unfractured and at ambient temperature. Lower rock strength will result when the rock is heated, fractured, or both.

3.1.4.5 What may happen if this parameter is not measured?

When rock strength parameters are unavailable, the potential for rock mass instability cannot be evaluated. Thus, unexpected failure of the underground workings may injure or kill people, and make it difficult or impossible to retrieve the waste. Furthermore, new fractures created may be potential leakage pathways that can adversely affect waste isolation.

3.1.4.6 Measurement conditions and potential instrumentation problems

Since rock strength is strongly dependent on the degree of welding and alterations in the tuff and on variations in porosity, lithophysal content, and fracture properties, significant variations in rock strength can be expected to occur at various localities throughout the repository. These factors will also cause rock strength parameters to be anisotropic. Rock strength parameters should be measured at numerous locations to account for spatial variability and anisotropy. Also, rock strength parameters used to design the repository workings and to predict repository behavior should be measured *in situ*. The volume of rock tested should encompass from a few to several cubic meters of rock which contain the geological heterogeneities expected to affect rock strength. Even doing that, it will be difficult to obtain rock strength measurements representative of the total repository rock mass.

3.1.5 Rock Modulus and Poisson's Ratio

Rock moduli (including Poisson's ratio) and viscoelastic constants describe the deformation behavior of rock under mechanical or thermomechanical stress. They are generally used to describe rock behavior at two scales: 1) small-scale, describing the behavior of small rock specimens (*i.e.*, a hundred to a few thousand cubic centimeters) which are typically intact, but may contain one joint; and 2) large-scale, describing the *in situ* behavior of larger rock masses containing several joints and involving a few to several cubic meters of rock.

On the small-scale, moduli of intact rock, over the short term, may deviate only slightly from the behavior of elastic materials. For that reason, parameters defined by the theories of elasticity are used in first-order calculations and as a fundamental part of the information in more complex modeling algorithms to compute behavior in stressed rock masses. In fact, a thorough understanding of the elastic characteristics of the rock will be essential to adequately model stresses and deformations in and around a repository in tuff. Modulus of elasticity (Young's modulus) and Poisson's ratio are the two most widely used and accepted fundamental parameters for the characterization of elastic materials in the range defined by Hooke's law (*i.e.*, where deformation is directly proportional to applied stress). Modulus of elasticity (E) is defined as the ratio of stress (σ) to deformation (strain, ϵ) for uniaxial stress (*i.e.*, $E = \sigma/\epsilon$); and Poisson's ratio (ν) is defined as the negative ratio of lateral deformation (ϵ_2) to axial deformation (ϵ_1) for an axial stress (σ_1) or applied load (*i.e.*, $\nu = -\epsilon_2/\epsilon_1$). Lame's constant ($\lambda$), modulus of rigidity or shear modulus (G), and bulk modulus or incompressibility (K) are other parameters defined by the theories of elasticity, and are related to Young's modulus and Poisson's ratio by the following expressions (Jaeger and Cook, 1979):

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)} \ ,$$

$$G = \frac{E}{2(1+\nu)} \ ,$$

and

$$K = \frac{E}{3(1-2\nu)}$$

These parameters are frequently used in three-dimensional analyses relating principal stresses and strains.

A material's behavior is called elastic if the strain returns to zero after a loading and unloading cycle. The relation between stress and strain need not be linearly proportional, nor does it need to follow the same path during unloading as during loading. Consequently, values of moduli representing slopes along a stress/strain curve, called tangent moduli, or values representing linear stress/strain lines drawn between the origin and individual points on the curve, called secant moduli, are sometimes used to more accurately represent moduli values of a material than the linearly proportional relation between stress and strain represented by Young's modulus. Whether a modulus is determined during loading or during unloading can also be significant. The actual behavior of certain rocks, such as intact tuffs, will generally be nonlinear during loading and unloading, and may not completely return to zero deformation after unloading. However, their behavior can still be reasonably approximated, within certain loading limits, by assuming elastic characteristics.

On the large-scale, deformational behavior of a rock mass to stress is influenced by discontinuities (*e.g.*, fractures, faults, lithophysae, and filling material), and by inhomogeneity and anisotropy. This is particularly true with tuff because: 1) rock mass characteristics vary with degree of welding and devitrification, 2) porosity and lithophysal content vary within any one tuff member and from member to member, and 3) the rock can be highly fractured. The term "modulus of deformation" (or deformation modulus), as opposed to modulus of elasticity (Young's modulus), is used in this report when discussing the stress/strain behavior of larger rock masses which do not closely follow elastic theory as a whole body, and/or have highly nonlinear stress/strain characteristics. Typically, deformation moduli and Poisson's ratio values increase, trending toward values for intact rock, as fractures close due to increased confining stress. An understanding of elastic properties of the intact rock, along with the deformation moduli and values of Poisson's ratio for larger masses, gives insight to the behavior of discontinuities within the rock; a knowledge that is critical to understanding the hydrology within a rock mass.

Creep deformation is one of the most important rock mechanics parameters in the assessment of long-term repository behavior. Viscoelastic constants describe the time-dependent deformation of rocks. These parameters can be empirically derived, or they can consist of linear rheological laws based on rheology models. Viscoelastic constants typically used are: 1) dynamic viscosity (expresses proportionality between shear stress and shear strain rate, which can be divided into two quantities—the rate of delayed elasticity and the rate of viscous flow), and 2) a measure of distortion, consisting of the elastic shear modulus and the amount of delayed elasticity (Goodman, 1980).

Even though fractures and other characteristics prevent rock from behaving elastically, Young's modulus and Poisson's ratio will provide valuable information useful to evaluating short-term stability of underground openings during the site characterization and construction phases. *In situ* measurements should be made during the site characterization phase to determine deformation moduli of larger rock masses, which are more representative of the rock that will be encountered during the repository construction and operation phases. Expected environmental conditions should be simulated as closely as practical. Because of the heterogeneity of tuff, Young's modulus, Poisson's ratio, and limited-volume deformation modulus should be included in the suite of parameter measurements that will progress into newly opened repository rock volumes during the construction phase. *In situ* stress and deformation measurements made as rock volumes relax during repository construction can also be useful parameters in determining deformation moduli.

It is likely that the elastic properties and deformation moduli of the near-field repository rock will change with time due to the elevated temperatures from the waste emplacement, and/or such other factors as dehydration, hydration, chemical changes, and stress changes. A thorough understanding of the hydrology through the repository system following closure will require a knowledge of the behavior of these properties and moduli as a function of time and environment. It is therefore recommended that they be remeasured within the repository system from time to time during the operations phase, along with the measurement of other parameters critical to repository hydrology (*e.g.*, permeability, fracture properties, *in situ* stress changes, and deformations and displacements). The long-term repository behavior evaluations should also include creep laws which describe time-dependent deformations of the rock mass.

Numerous parameters interact with the modulus of deformation and Poisson's ratio in rock. For example, modulus of deformation and Poisson's ratio relate stress to rock deformation, which causes change in fracture apertures and rock permeability. This, in turn, influences the movement of groundwater through fractures and can affect convective heat transfer. Rock moduli of deformation also affect the distribution of stresses surrounding repository openings (*e.g.*, high-stress concentrations may develop in the stiffer sections of the rock). Rock deformation moduli, including Poisson's ratio, are affected by various rock characteristics and environmental factors. Fracture characteristics such as frequency, aperture, and moisture content of filling materials affect deformation moduli. On the scale of a mined repository, fracture characteristics are not likely to be homogeneous. Therefore, deformation moduli can exhibit spatial variability throughout the repository. Furthermore, deformation behavior is likely to be anisotropic because fractures are anisotropic. Other factors influencing rock modulus of deformation and Poisson's ratio include porosity and lithophysal content, temperature, coefficient of thermal expansion, and the confining stresses acting on the rock. Rock maintained at elevated temperatures over long periods can possibly undergo changes in elastic properties.

Measurements of stress and deformation are used to obtain the deformation moduli. Consequently, the accuracy of deformation moduli is controlled by the accuracies with which stresses and deformations are measured. Measurements of deformations used in conjunction with deformation moduli are used to back calculate the stresses acting in the rock.

3.1.5.1 Normal parameter range

Price *et al.* (1984) report on mechanical tests conducted on thirty-five intact samples of Topopah Springs Tuff obtained at thirteen different stratigraphic levels ranging in depth from 147.7 to 390.3 m. Water saturated and water wet samples were deformed in compression at atmospheric confining pressure, room temperature, and a nominal strain rate of $10^{-5}\ \mathrm{s}^{-1}$. The ranges for Young's modulus and Poisson's ratio obtained during these tests were:

$$E = 13.0 \text{ to } 36.6\ \mathrm{GPa}\ ,$$

and

$$\nu = 0.13 \text{ to } 0.30$$

The wide ranges were attributed to large variations in the physical and mineralogic characteristics of the tuff.

Earlier mechanical tests conducted on Topopah Springs Tuff by Price *et al.* (1982) gave slightly higher values for Young's modulus and Poisson's ratio:

$$E = 22.9 \text{ to } 40.8 \text{ GPa} \ ,$$

and

$$\nu = 0.15 \text{ to } 0.33$$

These values were obtained from uniaxial tests on eleven core samples. Triaxial tests on four additional samples gave similar results with the caveat that "in general, the unconfined samples deformed in a brittle mode, while the confined samples exhibited macroscopic ductile behavior."

For comparative purposes Tillerson and Nimick (1984) have selected the values of elastic moduli provided in Table 11 to represent the four members of Yucca Mountain tuff. However, it should be noted that, to date, there have been no large scale tests on tuff from Yucca Mountain. Tillerson and Nimick (1984) have estimated that the *in situ* modulus of deformation for large rock masses will be in the order of one-half of the Young's Modulus values obtained in the laboratory.

3.1.5.2 Are these parameters site sensitive?

Rock moduli (including Poisson's ratio) are dependent on chemical composition, water content, porosity and lithophysal content, filling material, confining stress, and stress history. Therefore, they are site sensitive. Moreover, due to the heterogeneous nature of the tuff, moduli can vary within any specific tuff member.

3.1.5.3 Expected parameter variations during normal site operation

There may be variations in moduli as a function of temperature, as the rock is heated by thermal loading from the nuclear waste. There may also be variations with time, due to heating, geochemical changes, fracture aperture changes, and dehydration or hydration. For these reasons, sample measurements of rock modulus and Poisson's ratio should be continued until repository closure.

3.1.5.4 Parameter values that may signal trouble

Values for rock deformation moduli that may signal trouble are not known at present.

3.1.5.5 What may happen if these parameters are not measured?

Deformation moduli serve as input to the repository design and, in conjunction with creep laws, are used to predict rock behavior surrounding the repository and emplacement boreholes. If deformation moduli were unavailable, a faulty repository design could result in excessive deformation of the tunnels and emplacement holes. Excessive deformation can make retrievability difficult or impossible by causing instability of the repository tunnels or causing damage to the waste packages by excessive closure of the emplacement holes. Excessive deformation may cause backfilled boreholes to close, thereby binding canisters, extruding them from boreholes, or compressing waste packages and damaging them. Excessive deformation may also affect the transportation systems (*e.g.*, rails) used to handle the waste packages.

Table 11. Comparative values of Young's modulus and Poisson's ratio for Yucca Mountain tuffs (Tillerson and Nimick, 1984).

	Topopah Springs	Calico Hills	Bullfrog	Tram
E [GPa]	26.7 ± 7.7	8.1 ± 2.3	15.5 ± 4.5	21.8 ± 6.3
ν	0.14 ± 0.05	0.16 ± 0.06	0.19 ± 0.08	0.19 ± 0.07

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Displacement measurements used in conjunction with deformation moduli provide an integrated measurement of the stresses acting on the rock. Rock modulus and Poisson's ratio are necessary for translating rock deformation measurements into stress values within the rock mass. Even the use of rigid inclusion stressmeters requires some knowledge of these parameters for stress determination in rock such as tuff. The importance of determining deformation moduli by large-scale *in situ* testing, along with laboratory and borehole measurements, must be emphasized. Without large-scale measurements, deformation moduli that integrate discontinuity characteristics cannot be determined; and it is the network of discontinuities encompassing the intact rock matrix that controls the rock-mass response, not the rock fabric itself.

3.1.5.6 Measurement conditions and potential instrumentation problems

Rock deformation moduli can be affected by layering, by fractures and voids, by changes in the state of stress, and by the temperature of the rock. Tests in which deformation moduli are established should be performed under the same range of conditions (*i.e.*, temperature, stress, fracture and void characteristics, bedding planes) operating on the rock mass throughout the life of the repository. Rock moduli will be spatially variable throughout the repository because of the variability in local geologic conditions, and may change with time due to heating, geochemical changes, dehydration, or hydration.

3.1.6 Temperature

Temperature plays a role, either directly or indirectly, with nearly every measured repository parameter at one time or another. The most direct role of temperature is as a parameter in itself to monitor response to thermal loading and natural heating and cooling conditions in repository and test facility environments. Temperature measurements will be required at canisters, and in backfill, rock mass, air, and water to monitor responses to thermal loading from: nuclear waste; site characterization test emplacements; equipment (mining, drilling, lighting systems); ventilation, cooling, and heating systems; rock ambient conditions; and water flow, evaporation, and condensation.

Temperature is also a critical parameter in all thermal and thermomechanical response measurements. Thermal characteristics of repository rock media and engineered barrier materials should be measured under laboratory conditions with confirmatory measurements made *in situ* to account for variables not easily predicted or simulated in laboratory tests. These thermal characteristics are:

- thermal conductivity
- heat capacity
- thermal diffusivity (thermal conductivity divided by heat capacity).

The above parameters, along with the convective heat transfer parameter, are critical for modeling temperatures in the repository media to ultimately determine the thermomechanical response of the repository system. Their accurate determination requires accurate temperature measurements.

Thermal expansivity, or coefficient of thermal expansion, can be considered the principal thermomechanical response parameter. Thermal expansion provides the driving force for the other thermomechanical responses in the repository system. As with the thermal characteristics listed above, coefficients of thermal expansion should be determined by laboratory measurements and during *in situ* tests, and are dependent on accurate temperature measurements. Other measurements that are directly influenced by temperature and thermal expansivity include:

- initial stress
- stress changes
- deformation and displacements
- fracture and matrix permeability to steam, water, and air
- fracture aperture changes
- induced fracturing
- rock porosity
- rock decrepitation and spalling
- uplift

Certain rock property critical parameters are also a function of temperature, and in some cases are a function of the amount of time at elevated temperatures and, consequently, must be remeasured from time to time. These properties include:

- modulus of deformation
- Poisson's ratio
- rock strength

Modulus of deformation and Poisson's ratio are particularly important in modeling repository thermomechanical response and must be known over the full operating temperature range.

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Temperature also plays a role in hydrologic measurements. For example, fluid viscosity and vaporization are functions of temperature. During large-scale rock mass permeability tests (also referred to as macropermeability or ventilation experiments), evaporation and humidity levels are monitored and controlled by monitoring and controlling temperature levels.

The degree of water saturation in the unsaturated tuff will be influenced by rock temperature. Rock temperature will also influence fluid (liquid and gas) velocities within the rock matrix, fractures, and voids, and water inflow rates into repository openings (see Section 3.1.9, Convective Heat Transfer). In unsaturated media where relatively steep thermal gradients are present, there is a strong potential for convective heat transfer especially in the form of heat piping (*i.e.*, heat transfer caused by evaporation and condensation cycles) within the rock structure and in openings.

In geochemical measurements, temperature influences corrosion rate, dissolution rate, and sorption, as well as the fundamental groundwater chemistry parameters, pH, and Eh.

Temperature measurements can also signal sudden changes in local repository or test facility conditions. In this respect temperature changes can be used to detect cooling (or heating) from water inflow or sudden changes in water and moisture patterns. Rock decrepitation around heat sources can also be quickly detected by sudden changes in temperature patterns.

One of the more indirect, but important roles of temperature measurements, is in making thermal corrections to data obtained from other instrumentation. At elevated temperatures, like those in repositories or repository test facilities, it is not unusual for instrument thermal corrections to exceed output signals. Instruments requiring thermal corrections can include:

- extensometers for deformation measurements in rock and openings. (Corrections are required for rod or wire thermal expansion, and transducer temperature variations.)
- borehole strain gauges
- stressmeters
- geophysical tools
- hydrology pressure gauges
- geochemical instrumentation

Temperature is included as a critical parameter in all four repository phases. Its priority level is determined by the necessity for its direct measurement and monitoring, as well as its role as a parameter for thermomechanical response measurements. Though temperature is critical to other parameter measurements (*e.g.*, determining water viscosity for permeability measurements, influence on geochemical measurements, and instrument temperature corrections), these less direct influences are not part of the consideration for its priority level placement.

During the site characterization phase, temperature measurements will play a role in all the parameter measurements covered in the preceding part of this section. Tests requiring temperature measurements will simulate or exceed temperatures expected in the actual operating repository. In the site construction phase, the principal need for temperature monitoring will be for human comfort and safety. Typically, temperatures during construction will not greatly exceed rock ambient temperatures. During the site operation phase, temperature measurements will play a direct role in monitoring the repository response to thermal loading from high-level nuclear waste. Habitable areas will continue to be monitored for human comfort and safety. During the closure phase, temperature measurements will have a less significant role. Near-field temperature measurements may well be totally discontinued to facilitate repository sealing. However, temperature measurements may be continued by remote sensing and in surface experiments simulating repository conditions.

3.1.6.1 Normal parameter range

There are a number of constraints that can influence the maximum temperature limits at various locations within an operating repository in tuff. The first of these are the maximum allowable temperatures of the waste forms. A temperature limit of 350°C has been imposed to avoid degradation of Zircaloy cladding around spent fuel, and a temperature limit of 400°C has been imposed for commercial high-level waste (CHLW) glass, if that waste form should be used (O'Neal *et al.*, 1984). However, there are indications that if high-level waste is stored in vitrified glass form, the glass may be thermodynamically unstable and can eventually devitrify to a crystal form resulting in a highly soluble waste form (RHO, 1982, Vol. 2, Chap. II). To reduce this effect, the vitrified waste should not greatly exceed 300°C. Another consideration is that in the event that backfill materials containing bentonite are used in close proximity to waste canisters, the bentonite can irreversibly lose water at temperatures above 300°C.

Another constraint "is the 100°C maximum temperature limitation for the drift floor, a preliminary constraint based on the ability of men and equipment to reenter a storage room and retrieve waste canisters. The current value of 100°C for this constraint is somewhat arbitrary, but we believe it is a maximum value" (Johnstone *et al.*, 1984). This constraint is dependent on such factors in the repository design as "canister standoff distance" from the drift floor (for vertical emplacement) or from the drift wall (for horizontal emplacement), and whether rooms are ventilated, unventilated, or backfilled. This 100°C limitation can be a controlling factor in optimizing the repository gross thermal loading (GTL). Another closely related constraint influenced by similar repository design factors is a peak temperature limitation of 150°C at 1 m from the canister borehole during the first 110 years following the start of repository operation (Peters, 1983).

St. John (1985) has reported on the results of preliminary calculations of temperatures in welded tuff for waste canisters emplaced in vertical boreholes. These calculations indicate that temperatures at canister borehole walls will peak at about 215°C for ventilated drifts and about 240°C for unventilated drifts. The peak temperatures occur after 3 to 4 years in the ventilated drifts and after 9 years in the unventilated drifts. For the ventilated drift analysis, the drift perimeter was maintained at 30°C. Peters (1983) has reported that canister borehole-wall peak-temperatures for horizontal emplacement are roughly the same as peak temperature for vertical emplacement assuming the same gross thermal loading and canister thermal dissipation

The average ambient rock temperatures are given by Johnstone *et al.* (1984) for potential repository units in Yucca Mountain tuff as 26°C for Topopah Springs, 30°C for Calico Hills, 38°C for Bullfrog, and 41°C for Tram. Ventilation may provide some cooling, however, even considering the most likely potential site in the welded tuff of the Topopah Springs Member it is unlikely that minimum temperature will go below 20°C during any repository phase. Therefore, it is probably safe to assume that the normal temperatures that will be encountered over the life of a repository in tuff will range from a minimum of 20°C in any drift to a maximum of 350°C within the waste form, with the following caveats: 1) the maximum allowable temperature of the waste form might be reduced, and 2) during site characterization tests, some temperatures may be driven to extremes well above the maximum temperatures expected within the waste form (perhaps to 500°C, or more).

3.1.6.2 Is this parameter site sensitive?

Temperature will be dependent on thermal conductivity, heat capacity, initial ambient temperatures, and hydrologic conditions; all of which can vary from one site to another. However, engineering considerations such as gross thermal loading, individual canister thermal output, backfill emplacement, and cooling will probably override the inherent site sensitivities.

3.1.6.3 Expected parameter variations during normal site operation

Canister and borehole wall temperatures will peak sometime within the first ten years of waste emplacement, depending on the waste material, its cooling period prior to emplacement, and repository design considerations such as horizontal or vertical emplacement, ventilation and backfilling. A maximum relative gross thermal loading of 57 kW/acre was determined for Topopah Spring Tuff, so that drift floor temperature reaches 100°C 110 years after waste emplacement (Johnstone *et al.*, 1984). At 50 years the drift floor temperature will be between 95 and 97°C. Far-field temperatures at 15% of the distance between the repository and the surface will peak at approximately 1000 years, and at 85% of the distance to the surface, peak temperatures will be reached in approximately 10,000 years (Johnstone *et al.*, 1984).

In the unsaturated tuff, convective heat transfer (especially in the form of heat piping through the rock matrix, fractures, and voids) can provide a significant heat transfer mechanism. In the repository case, heat piping refers to the transfer of heat to water during vaporization followed by the movement of that vapor through the rock matrix, fractures, or voids (such as lithophysae) to a cooler rock volume where it is recondensed, thus transferring its heat to that cooler rock. Many of the preliminary rock temperature calculations have not included convective or radiant heat transfer and, therefore, probably result in near-field temperatures that are higher than may actually be encountered.

3.1.6.4 Parameter values that may signal trouble

Any measured temperature value that does not fall within a predicted range at any point in the repository may signal trouble such as:

- Excessive canister temperatures. Maximum temperatures depend on the waste form, but in the case of Zircaloy clad spent fuel, maximum acceptable temperature will probably be about 350°C.
- Excessive temperatures in habitable locations. Temperatures above established values can indicate dangerous cooling and ventilation system failures.

Sudden changes in temperature, even though they may be small, may also signal trouble. These changes can be indicative of such phenomena as:

- Rock decrepitation or spalling, which can be particularly significant around waste canisters not protected by borehole liners or backfill. Decrepitated or spalled rock can act as a thermal insulator, causing a rise in canister temperatures.
- Cooling and ventilation system failures.

3.1.6.5 What may happen if this parameter is not measured?

Temperature is truly one of the critical parameters in repository measurements. Without knowledge of this parameter, thermal characteristics, and thermomechanical response parameters are meaningless. Most hydrological and geochemical measurements in a repository environment are temperature dependent. Nearly all *in situ* instrumentation also requires temperature correction.

3.1.6.6 Measurement conditions and potential instrumentation problems

The relatively high temperatures that might be encountered in repository drifts following waste emplacement may require special cooling or design considerations for some instrumentation-support electronics (*e.g.*, thermocouple temperature references, and signal amplifier).

3.1.7 Expansivity

Expansivity as a repository critical parameter includes such characteristics as coefficients of thermal expansion, expansion due to changes in confining pressure, and expansion due to hydration of clays (*e.g.*, bentonite) used in backfill mixtures. This section of the report concentrates on the role of thermal expansion in repository measurements. Expansion due to changes in confining pressure is covered in Section 3.1.5 under the topic of Rock Modulus and Poisson's Ratio. Expansion due to the hydration of clay and rock backfill mixtures, their sealing capabilities, and any stresses resulting from their expansion, should be thoroughly studied during the site characterization phase; and will depend on site-specific engineering configurations and requirements.

The coefficient of thermal expansion describes the dimensional change experienced by a material with change in temperature. In tuff, as with other rock types, this can be affected by anisotropic characteristics, heterogeneity of the rock throughout the repository, and discontinuities within any specific rock volume. Hydrous mineral phases present in some tuffs can also influence expansivity as a function of temperature and, very likely, as a function of the amount of time that the rock is maintained at an elevated temperature. Confining pressure will also influence thermal expansion of the tuff. In this sense, there is an interaction between coefficient of thermal expansion and such other parameters as modulus of deformation, Poisson's ratio, porosity, and degree of microfracturing.

The coefficient of thermal expansion is one of the basic thermal properties of a material. Thermal expansion can also be considered as the basic thermomechanical driving force that couples temperature change to other thermomechanical response parameters. In a repository environment, these other parameters can include:

- initial *in situ* stress
- stress changes
- deformation and displacement
- permeability
- fracture aperture changes
- induced fracturing and fracture growth
- rock porosity
- rock decrepitation and spalling
- uplift

Coefficients of thermal expansion will be used in testing, modeling, and analysis throughout the life of the repository. However, since values and characteristics for this parameter should be completely determined by laboratory and *in situ* measurements during the site characterization phase, it is listed as a critical parameter during that phase only, with the consideration that some tuffs exhibit a temperature/time expansivity characteristic caused by the presence of variable amounts of hydrous mineral phases. If a repository is constructed within a tuff that exhibits this property, periodic measurements should be made throughout the operating phase to ensure that dehydration from radiogenic heating does not cause excessive contraction of repository rock, significantly reducing its structural integrity.

3.1.7.1 Normal parameter range

Table 12 summerizes the unconfined linear thermal expansion coefficients obtained from measurements on 21 samples of devitrified welded tuffs collected from three locations at the Nevada Test Site (hole Ue25 #1 on the flanks of Yucca Mountain, well J-13, and within the G-tunnel complex beneath Rainer Mesa). Fourteen of these samples with analyzed final porosities of from 8 to 26% were fairly uniform in behavior to 200°C, with unconfined linear expansion coefficients of $8.9 \pm 1.6 \times 10^{-6} {}^{\circ}C^{-1}$ (Lappin, 1980).

"Because of the presence of variable amounts of hydrous phases, such as clays, zeolites, glass and opaline silica, three temperature ranges must be defined for the thermal expansion behavior of the tuffs from Yucca Mountain: pretransition, transitional, and post transition. For the welded, devitrified Topopah Springs Member, the transitional behavior is caused by a mineralogic phase change, while mineral dehydration causes the variation in tuffs containing significant quantities of hydrous minerals" (Tillerson and Nimick, 1984).

The thermal expansion characteristics of the devitrified, densely welded tuffs of the Topopah Springs Member change above about 200°C, because of variations in amount of cristobalite present. Lappin (1980) explains that cristobalite inverts over some temperature range from a low-temperature tetragonal form (α cristobalite) to a cubic form (β cristobalite), which is stable at high temperatures, causing a volumetric increase during this mineralogic phase change. The resulting nonlinearity is seen as an increased coefficient of thermal expansion between the temperatures of 200 and 350°C. This effect is also apparent in the thermal expansion coefficients given in Table 12 for other devitrified welded tuffs from the Nevada Test Site. One additional note is that the $\alpha-\beta$ cristobalite transformation shows a heating rate-independent hysteresis, with transformation temperatures 16 to 40°C lower during cooling than during heating (Lappin, 1980; Sosman, 1965). Linearized thermal expansion coefficients for Topopah Springs tuff are given in Table 13 along with the coefficients for three other Yucca Mountain tuffs.

The presence or absence of cristobalite in welded tuff appears to have a major effect on thermal expansion only at temperatures above 200°C. Even at high waste emplacement densities, this would be of potential concern only in the very-near-field environment. It also appears that porosity, *per se*, and lithophysal porosity, in particular, have no impact on the expansion behavior of the densely welded Topopah Springs Member (Lappin, 1980; Tillerson and Nimick, 1984).

Because of the presence of hydrous mineral phases, the Calico Hills, Bullfrog, and Tram tuffs exhibit an equivalent negative thermal expansion during transitional dehydration. During con-

Table 12. Linear thermal expansion coefficients from 21 samples of devitrified welded tuff (Lappin, 1980).

Temperature Intervals [°C]	Coefficients of Linear Thermal Expansion [$10^{-6} {}^{\circ}C^{-1}$]	
	Average	One Standard deviation [1σ]
amb-100	6.9	±1.5
100-200	11.3	±2.6
amb-200	9.3	±1.8
200-300	17.6	±6.9
amb-300	12.3	±3.5
300-400	15.0	±3.4
400-500	15.3	±5.3
amb-500	13.5	±1.9

Table 13. Thermal expansion coefficients of Yucca Mountain tuffs [10^{-6}°C^{-1}] (Johnstone *et al.*, 1984; Tillerson and Nimick, 1984).

	Topopah Springs	Calico Hills	Bullfrog	Tram
Average Case				
Pretransition (Temp. Range,°C)	10.7 ± 1.7 (to 200)	6.7 ± 3.7 (to 100)	8.3 ± 1.4 (to 100)	8.3 ± 1.4 (to 100)
Transitional (Temp. Range,°C)	31.8 (200–350)	−56.0 (100–150)	−12.0 (100–125)	−12.0 (100–125)
Post transition (Temp. Range, °C)	15.5 ± 3.8 (350–400)	−4.5 ± 4.0 (150–300)	10.9 ± 0.8 (>125)	10.9 ± 0.8 (>125)
Limit Case				
Pretransition (Temp. Range,°C)	14.1 (to 200)	−0.4 (to 100)	5.2 (to 100)	5.2 (to 100)
Transitional (Temp. Range,°C)	53.6 (200–350)	−115.0 (100–150)	−20.0 (100–125)	−20.0 (100–125)
Post transition (Temp. Range,°C)	23.1 (350–400)	−9.3 (150–300)	9.4 (>125)	9.4 (>125)

fined measurements, the effects of increasing confining and fluid pressures were to elevate the temperatures at which dehydration took place and to make expansion more linear than in unconfined tests. Though it is apparent that contraction takes place during dehydration at transitional temperatures (Table 13), detailed measurements have not yet been made of the combined time and temperature effects on the transitional characteristics.

3.1.7.2 Is this parameter site sensitive?

Because of the anisotropy and heterogeneity of tuff within any stratigraphic unit and from one unit to another, and because of dependence on the degree of saturation, coefficients of thermal expansion are spatially variable and site sensitive.

3.1.7.3 Expected parameter variations during normal site operation

Tuffs containing hydrous mineral phases can undergo time-temperature dependent changes due to dehydration (and rehydration) at transitional temperatures. These effects, which are influenced by confining and fluid pressures, should be thoroughly studied during site characterization and well understood before entering the site construction phase. The actual parameter variations within the repository system, however, will occur during the site operations phase as a result of radiogenic heating from the emplaced waste canisters.

3.1.7.4 Parameter values that may signal trouble

Excessive contraction during transitional temperatures in tuffs containing hydrous phases can reduce repository and borehole structural integrity. Current information indicates that this should not be a significant problem above the water table in the Topopah Springs Member.

3.1.7.5 What may happen if this parameter is not measured?

Determining this parameter is critical to early modeling of the thermomechanical and hydrologic response of the repository system. Direct measurements of other thermomechanical responses (stress changes, deformations and displacements, permeability, fracture aperture changes, porosity and microfracturing, and

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uplift), along with temperature and temporal effects, should be used to confirm the calculated responses from thermal expansion coefficients. Measurements of these types are, conversely, used in determining the coefficients of thermal expansion. Larger-scale *in situ* tests, in addition to laboratory tests on smaller samples, should be used to adequately determine the rock mass expansivity properties. Tillerson and Nimick (1984) point out that in some cases measured stress changes in large scale tests have been approximately 40% of the stress changes calculated by using laboratory-derived expansion values obtained from measurements on relatively small, intact samples. However, they attribute this to likely differences between rock mass deformation modulus and matrix elastic modulus rather than to differences in thermal expansion.

3.1.7.6 Measurement conditions and potential instrumentation problems

The biggest problem in measuring the coefficients of thermal expansion within a tuff horizon may result from the anisotropic and heterogeneous rock characteristics and time dependent variations at transitional temperatures. Differences between vertical and horizontal confining pressures may also affect the directional characteristics of this parameter. It will probably be necessary to make a number of multiple-axis, *in situ* measurements over a significant volume of the candidate rock to obtain representative parameter values. Another problem will be in obtaining representative thermal expansion coefficients for the strata above and below the candidate horizon with minimum penetration into those regions.

3.1.8 Thermal Conductivity, Heat Capacity, and Diffusivity

Any two of the three parameters: thermal conductivity, heat capacity, or thermal diffusivity are critical in determining the rate of heat transfer from high-level nuclear waste material and the heat storage capacity of the media surrounding the waste canisters. The third parameter is completely defined by the other two. These properties ultimately influence the waste, canister, backfill, and rock temperatures; and, consequently, they influence the thermomechanical response of the repository system.

Thermal conductivity, heat capacity, and thermal diffusivity are interrelated, as shown in the following expression:

$$D = \frac{k}{cd} \quad ,$$

where:

D = thermal diffusivity
k = thermal conductivity
c = specific heat
d = density
cd = heat capacity

Thermal conductivity (k) represents the time rate of heat transfer through a unit thickness, across a unit area for a unit temperature gradient. The specific heat (c) of a substance is the heat per unit mass per degree change in temperature, and heat capacity (cd) is the heat per unit volume per degree change in temperature.

It is assumed that the engineered materials (waste form, canisters, backfill, etc.) can be designed to meet their heat transfer needs. When considering measurement requirements, the critical parameters are the thermal conductivity, heat capacity, and thermal diffusivity of the rock mass. These parameters will be influenced by porosity, fracture density and aperture, water content of the rock, and other hydrologic conditions that can vary throughout the repository rock volume, and, consequently, which may be difficult to simulate in small-scale laboratory experiments. It will probably be necessary to perform a number of scattered *in situ* heated rock tests, each with the capacity to heat rock volumes of the order of tens of cubic meters, to adequately encompass the variables. Heated rock experiments to determine these parameters *in situ* are relatively simple in concept. Basically, they require a well-controlled heat source (*e.g.*, such as an electric heating unit) positioned in the rock and an array of temperature sensors located in the rock volume surrounding the heat source at various distances from it. Interpreting the results from these experiments, on the other hand, is not necessarily simple.

A number of other critical parameters interact with the three basic thermal parameters by having an influence on thermal conductivity, heat capacity, and thermal diffusivity, or *vice versa*. Accurate temperature measurements are extremely important in determining these three parameters, and, in turn, the three parameters directly influence temperatures throughout the repository system. In some cases these parameters are also temperature and time/temperature dependent. In the unsaturated tuff, convective heat transfer can interact dramatically with the three basic thermal parameters in the sense that significant quantities of heat can be transferred by evaporation and recondensation cycles coupled with vapor and water transport through the rock mass. Since the rock mass thermal properties directly influence temperature throughout the rock, they also influence thermal expansion which, in turn, influences rock stresses, and displacements and deformations. Rock strength also interacts with thermal properties in the form of degradation at high temperatures. Conversely, thermomechanically induced fractures, and decrepitation and spalling can influence thermal properties.

Thermal properties will be used in modeling and data analysis throughout the life of the repository. However, since these properties, under defined conditions, should be completely determined by laboratory and *in situ* measurements during the site characterization phase, they are considered critical parameters of primary importance only during site characterization. If conditions in the repository rock should vary in a manner not predicted during site characterization (*e.g.*, due to extensive dehydration, hydration, or decrepitation and spalling), it may become necessary to make verification measurements of the thermal properties during the construction or operating phases.

3.1.8.1 Normal parameter range

This section summarizes the parameter ranges for thermal conductivities and heat capacities of tuffs in general, and Yucca Mountain tuffs in particular, along with values of other rock mass properties that directly influence these thermal parameters. Thermal diffusivity is not specifically covered, but can be computed from thermal conductivity and heat capacity using the equation given in section 3.1.8. Units are m^2/s.

Published values for saturated thermal conductivities of welded tuffs range from 1.4 to 2.5 W/m°C and from 1.2 to 1.9 W/m°C for zeolitized nonwelded tuffs. Some of the data were obtained at pressures and temperatures above ambient, and, therefore, upper values for the ranges are probably slightly higher than would apply at ambient conditions (Tillerson and Nimick, 1984).

Thermal conductivity of tuff is dependent on porosity and degree of saturation, and is sensitive to variations in mineralogy. Grain density has been successfully used in calculating the conductivity to reflect the influence of mineralogy. In general, zero-porosity or matrix conductivity for a mineralogically homogeneous tuff layer, combined with porosity and degree of saturation, can be used to estimate *in situ* conductivity by using the following assumptions regarding lithophysal zones and rock joints (Tillerson and Nimick, 1984). Below the water table, lithophysae and joints can be treated as saturated pores. In the Topopah Springs Member above the water table, lithophysae can be treated simply as additional air-filled porosity. It may also be assumed that virtually all joints are air-filled in the Topopah Spring Member even though the matrix may be near full saturation. Under this assumption, the fully saturated ambient temperature conductivity of nonlithophysal tuff may be reduced from 2.1 to 1.8 W/m°C, or by about 15%. A similar but smaller reduction is also possible in conductivity of dehydrated rock mass (Tillerson and Nimick, 1984).

Table 14 summarizes the thermal parameters and the associated physical properties that influence them for the four Yucca Mountain tuffs of interest. Note that parameters given in this table do not reflect the fact that, at temperatures near the boiling point of water, apparent conductivities and heat capacities will be artificially high because of the heat of vaporization required to transform liquid water to a vapor phase. This point is also discussed briefly under the topic of Convective Heat Transfer, Section 3.1.9.

Tillerson and Nimick (1984) have reported that calculated values of specific heat for Topopah Springs tuff range from 0.84 to 1.30 J/g°C, depending on porosity and saturation, and assuming a constant value of 0.84 J/g°C for the silicate mineral assemblage. The calculated values are somewhat dependent on mineralogy (grain density). Calculated values of heat capacity (specific heat × density) given in Table 15 show the strong dependence on both porosity and degree of saturation. The following relation was used for these calculations:

$$(cd)_{bulk} = d_g\,(1 - \phi)c_s + (cd)_w\phi S$$

where:

$(cd)_{bulk}$ = rock mass heat capacity [J/cm^{3}°C]
d_g = grain density [g/cm^3]
c_s = specific heat of silicates [0.84 J/g°C]
$(cd)_w$ = heat capacity of water [4.18 J/cm^{3}°C]
ϕ = porosity
S = degree of saturation

Note: capacity of air is assumed to be 0.0 J/cm^{3}°C.

Table 14. Thermal parameters and associated physical properties of Yucca Mountain tuffs (Tillerson and Nimick, 1984).

Property	Topopah Springs	Calico Hills	Bullfrog	Tram
Porosity	0.17±0.09	0.32±0.02	0.23±0.03	0.19±0.03
Grain density [g/cm^3]	2.55±0.03	2.40±0.02	2.59±0.02	2.64±0.04
Saturation	0.8	1.0	1.0	1.0
Saturated bulk density [g/cm^3]	2.29	1.95	2.22	2.33
Dry bulk density [g/cm^3]	2.12	1.63	1.99	2.14
Saturated thermal conductivity [W/m°C]	1.8±0.4	1.4	2.0±0.1	2.2±0.1
Dry thermal conductivity [W/m°C]	1.6±0.4	1.0±0.05	1.4±0.2	1.6±0.2
Heat capacity [J/cm^3°C]	2.18	2.72	2.64	2.59

Table 15. Calculated heat capacities for saturated and dry tuff rock masses as a function of porosity and grain density (Tillerson and Nimick, 1984).

	Rockmass Heat Capacity [J/cm^3°C]			
Grain density	2.65 g/cm^3		2.38 g/cm^3	
Porosity	Saturated	Dry	Saturated	Dry
0.0	2.22	2.22	2.01	2.01
0.1	2.43	2.01	2.22	1.80
0.2	2.59	1.76	2.43	1.59
0.3	2.80	1.55	2.64	1.38

3.1.8.2 Are these parameters site sensitive?

Because of the heterogeneous nature of tuff and variations in porosity and degree of saturation, thermal properties can vary from one site to another, among stratigraphic units, and within any single unit.

3.1.8.3 Expected parameter variations during normal site operation

Thermal properties are temperature dependent and they can be influenced by changes in rock fracture characteristics and water content of the rock during normal site operation. However, parameter variations due to these phenomena should be thoroughly determined during the site characterization phase. The most dramatic variation in thermal properties will probably be associated with rock drying due to dehydration of hydrous phases within the tuff and the evaporation of free water. Another variation in thermal properties can occur with rock decrepitation or spalling. This can be most significant around waste canisters not protected by liners or backfill, where decrepitated and spalled rock can act as a thermal insulation resulting in a waste-form temperature rise. This phenomenon should also be simulated and modeled during site characterization.

3.1.8.4 Parameter values that may signal trouble

Changes in thermal conductivity and rock heat capacity can signal trouble, such as rock decrepitation, spalling, or excessive dehydration. However, these parameters will probably be monitored indirectly during site operation by monitoring temperatures at critical locations within the repository. Monitoring systems incorporating established temperature maximums, determined by the repository system design, should provide adequate indication to signal any trouble resulting from unexpected changes in thermal properties.

3.1.8.5 What may happen if these parameters are not measured?

Thermal properties of the tuff are critical in determining the rate of heat transfer from waste packages. Without representative values, waste, canister, backfill, rock, air, and water and vapor temperatures within the repository system cannot be adequately modeled. Representative thermal properties of rock above and below the repository horizon must also be determined to completely model repository far-field temperature response and, consequently, long-term thermomechanical response. This modeling is particularly important to ensuring that nuclear waste forms do not exceed certain maximum temperatures that will adversely influence radioactive release rates.

3.1.8.6 Measurement conditions and potential instrumentation problems

Anisotropic and heterogeneous characteristics, along with water content variations in the rock, and other hydrological conditions, may require a number of *in situ* measurements to obtain representative values for thermal properties in the repository rock and surrounding media. Laboratory tests can help in determining these properties, however, it will be nearly impossible to simulate all of the *in situ* conditions in the laboratory. Consequently, relatively large-scale tests, covering tens of cubic meters of rock volume, will be required at *in situ* test facilities. Though simple in concept, these tests require the emplacement of relatively large well-controlled heaters (on the order of a few kilowatts per simulated canister), and a sufficient number of instrumentation boreholes surrounding the heater to adequately monitor the temperature distribution in the rock.

3.1.9 Convective Heat Transfer

In this report, the topic of convective heat transfer includes the transfer of heat by thermally induced circulation of fluids (either liquid or gas), exchange of heat by fluid vaporization or condensation, or a combination of these phenomena. Convective heat transfer *per se* does not include direct heat transfer by the natural water infiltration through the rock formation (*i.e.*, percolation), or by natural flow of water within and between hydrostratigraphic units. It may be difficult, and possibly unnecessary, to completely distinguish between the effects of natural flow and the effects of convective heat transfer during *in situ* measurements to determine net heat transfer from waste canisters. However, from the computer modeling point, it will undoubtedly be necessary to consider the effects of each individual heat transfer component to model canister and repository temperatures. The importance of thermal conductivity, heat capacity, and thermal diffusivity in this regard has been discussed in Section 3.1.8.

Convective heat transfer probably will not contribute significantly to the overall heat transfer in a saturated rock formation with low porosity and low permeability, and where hydrostatic pressures are high enough to prevent vaporization. However, in porous, permeable, saturated hydrostratigraphic units, or where fluid flow paths (channels) exist between such hydrostratigraphic units, convective circulation can not only contribute to heat transfer, but can also provide a mechanism for the transport of radionuclides. Convective fluid velocities in saturated rock are directly related to the intrinsic permeability of the rock matrix and fracture system as discussed in Section 3.3.2, Permeability, and the volume of water available for convective flow is directly related to porosity (Section 3.3.5, Porosity and Distribution of Pore Sizes). The driving forces behind convective flow are provided by heat-induced variations in water density, thermal expansion, and, under proper pressure and temperature conditions, pressures caused by boiling, and heating of vapor (or, conversely, by reduced pressures resulting from the cooling of gaseous-phase water, and condensation). Heat transfer can also occur by vaporization of water from rock adjacent to repository openings. This mechanism can provide considerable cooling in open waste-storage boreholes in saturated permeable tuff (Klasi *et al.*, 1982; Klasi *et al.*, 1982a). However, since the primary candidate horizon for a repository in tuff is located in the unsaturated region of the Topopah Springs Member, well above the water table, heat transfer in the far-field saturated region (*i.e.*, below the water table) will have negligible influence on repository temperatures for a considerable number of years.

On the other hand, for a repository located in partially saturated tuff, convective heat transfer can have a significant influence on waste canister and near-field rock temperatures, and on near-field hydrology. Temperatures can be influenced by several convective heat transfer mechanisms in the unsaturated tuff, including: thermally induced convective flow of fluids (liquid and gas phase) through pores, fractures, lithophysal voids, and man-made openings; heat piping; and evaporation of water from rock into repository openings.

When considering convective heat transfer, it must be kept in mind that when more than one fluid or fluid phase is involved in convective flow within rock pore spaces, the flow rates of the fluids interact with one another. See Section 3.3.3, Relative Permeability, for a discussion of this phenomenon. Convective heat transfer can be further complicated by "heat piping," a term that not only includes fluid flow, but also the transfer of heat by vaporization and condensation. Basically, heat piping is a thermal cycle initiated when heat is transferred to water during its evaporation. The evaporated fluid convectively moves to a cooler environment where it recondenses, transferring heat to that environment, The recondensed fluid then flows back to the original heat source to complete the cycle.

In the case of a repository, heat piping refers to a sequence of events that begins with the transfer of heat by vaporization of water (boiling or evaporation), such as the transfer of heat from radiogenically heated waste canisters or from rock heated by waste canisters. Since the latent heat of vaporization is 5.4 times greater than the amount of heat required to raise an equivalent mass of water from 0 to 100°C at atmospheric pressure, the amount of heat that can be transferred by vaporization (or condensation) is quite significant relative to the heat capacity of liquid-phase water, and, possibly, relative to the heat transferred by convective circulation of the liquid-phase water (depending on the degree of saturation, rock permeability, porosity, and fracture characteristics). The second step in heat piping involves vapor (*i.e.*, gas-phase water) movement away from the heat source to a cooler volume by convective flow, or as a result of pressure from vaporization and thermal expansion of the vapor. Near repository openings, some (or all) of the vapor can escape into open space where it can be partially (or completely) removed from the repository system by ventilation, while vapor remaining in the rock formation moves through permeable rock toward cooler zones. In either case, heat is removed from the location where vaporization took place. Although heated vapors generally move upward, horizontal or downward movement can also take place under various conditions that can be encountered in a repository. The third step involves the transfer of heat from the vapor back into a cooler volume of the repository system by the recondensation of those vapors not removed from the system. This recondensation can take place within the rock formation, boreholes, or in other voids or openings. The net result is that heat is transferred (primarily as a function of the latent heat of vaporization) from where the water vaporizes to where it recondenses.

In a conventional closed-system heat pipe, condensate flows back to the heat source by gravitational force or capillary pressure to complete the fluid flow cycle. In the more complex repository environment, other flow mechanisms created by local changes in hydrology due to near-field heating and convective fluid flow can also play a part in circulating water back toward the heat source. Though the fourth step in a closed heat piping cycle involves recirculation of condensate back to the heat source, this is not a necessary condition during heat piping in a repository. Water can be replenished to the heat source from heat piping condensate, from origins completely isolated from the condensate, or from a combination of these. Heat piping can also be a transient phenomenon where vaporized water is not replenished at all, is only partially or slowly replenished, or is replenished in quasi-periodic bursts. In any case, convective heat transfer effects will be time variant as temperature fields move outward in the repository formation.

Because heat piping in a repository environment depends on the latent heat of vaporization of water, it can potentially transfer significant amounts of heat through the porous, permeable tuff and in boreholes near waste canisters where high thermal gradients exist. For example, vertical boreholes used for canister emplacement can act as nearly ideal closed-system heat pipes under certain conditions (*i.e.*, when annular space between canisters and borehole walls and space above canisters are left open and connected; when there is a sufficient thermal gradient between the emplacement zone and the upper part of the borehole; and when the proper amount of water is available within the borehole). Basically, heat from a canister (or canisters) evaporates water in the lower part of a borehole. This vapor-phase water is convectively transported upward into surroundings cool enough for it to condense into droplets on the borehole wall (and/or cover, if the borehole is closed), thus transferring heat from the canister region to rock surrounding the upper part of the borehole. Condensate accumulates until the droplets become heavy enough to break free and fall or run back down into the heated zone to again be evaporated. It should be noted that even if there is insufficient water for heat piping to take place, heat transfer by convective currents in a similar vertical emplacement configuration can still be significant, though somewhat less.

Convective heat transfer involving heat piping similar to that described in the preceding paragraph was observed during experiments in granite at Stripa, Sweden, where electrically heated canisters were used in vertical boreholes to simulate thermal loading from stored waste (Cook and Hood, 1978). Another heat piping phenomenon was observed both at Stripa and in the BWIP experiments at Hanford, when small quantities of water were captured in closed-bottom tubes in which thermocouples were inserted. A boiling and condensing cycle was created within the tubing, causing thermocouple readings to oscillate erratically between 100°C and the valid temperatures above boiling. This continued until the tubes were cleared of the moisture (Wilder *et al.*, 1982; Binnall and McEvoy, 1985). Convective heat transfer with heat piping was also observed in vertical boreholes at Stripa where strings of thermocouples were installed (but not in tubing) to measure temperature profiles in the granite during the experiments. This was observed even in boreholes that were backfilled with sand.

Convective heat transfer involving heat piping cycles can also occur when canisters are emplaced in long, horizontal boreholes under conditions similar to those mentioned previously for vertical emplacement. The principal differences are that the convective flow of the evaporated water will probably be less effective down the horizontal length of the borehole, and the condensed water that accumulates at the cooler end (or ends) of the borehole must flow back toward the canister-heated zones along the borehole wall and within the adjacent permeable tuff by capillary pressure alone (*i.e.*, without the aid of gravity). Convective heat transfer within the horizontal borehole and surrounding rock can also cause a general upward shift of isotherms.

For the most part, convective heat transfer anywhere in the repository system (with or without heat piping) can provide a positive influence on the reduction of canister and very-near-field temperatures by facilitating a more rapid and wider distribution of the radiogenic heat. As an additional example, properly engineered closed-system heat pipes placed down the central axis of waste canisters could even be used to reduce peak temperatures in the waste by distributing heat to the ends of the canisters, which, in turn, could be designed to further dissipate the heat.

On the negative side, convective flow can act as a transport mechanism for radionuclides and corrosive chemical species. This topic, Volatility and Gaseous Diffusion of Radionuclide Chemical Species, is discussed in Section 3.4.5 of this report. Corrosive chemistry natural to the repository or formed by radiolysis is discussed in Section 3.4.6, Canister and Support System Corrosion.

Convective flow can also influence near-field hydrology in the partially saturated tuff. Aside from direct influences on natural flow patterns by convective circulation, convection can also cause localized variations in the degree of saturation within the rock formation. This can be particularly significant under heat-piping conditions because of the relatively large changes in saturation that can occur at locations where evaporation and condensation take place. As previously mentioned in this section and discussed in more detail in Section 3.3.3, Relative

Permeability, when liquid- and gas-phase fluids both exist within the pore space of a rock, the rate at which one fluid flows through the rock is influenced by the presence of the other. Hence, natural hydraulic flow is further disturbed by changes in the degree of saturation, as are vapor-phase flow rates. In the extremes, localized zones can become either irreducibly saturated (see Section 3.3.4.1), or totally saturated. A zone that is only partially saturated under undisturbed conditions can become saturated if, for example, a sufficient amount of condensate from heat piping should combine with a sufficient amount of water from natural infiltration. In this case, the hydrologic flow in that zone would change from an unsaturated flow, dominated by capillary pressures, to a saturated flow. For example, open fractures would become hydraulic conduits for saturated flow rather than barriers to capillary flow. If a saturated front should form in the rock above or surrounding a heat source, gas-phase flow through the rock would be impeded or stopped.

Convective heat transfer is considered to be a critical parameter in unsaturated tuff during the site characterization phase when it will be important to determine and understand its influence on the repository response to thermal loading, and to provide data for the development and verification of models used to predict repository temperatures, hydrologic flow, and radionuclide transport. Measurements should also be made during the operations phase to confirm the repository response.

Convective heat transfer can interact with a number of the other critical parameters. The most direct interaction should probably be considered to be the interaction with temperature, since temperature directly influences convective heat transfer, and convective heat transfer has a direct influence on temperature fields in the rock formation, openings, and waste canisters. The following other critical parameters interact with convective heat transfer in the sense that convective flow, which can include heat piping, requires openings and channels through which flow can take place:

- permeability (fracture and matrix)
- porosity and distribution of pore sizes
- geologic variables (especially lithophysal characteristics)
- fracture properties
- induced fractures

The parameters just listed also interact with convective heat transfer in the sense that they can affect the supply of water available for heat piping and liquid-phase convective circulation, as can the following parameters:

- water infiltration rate
- groundwater recharge and discharge locations and rates
- water saturation
- water potential
- saturation characteristics
- relative permeability
- fluid velocity
- water inflow rate

Convective heat transfer, in turn, can have an influence on all but the first two of these latter parameters.

Among the most important interactions to thoroughly understand are the influences that convective heat transfer can have on *in situ* measurements used to determine values for thermal conductivity, heat capacity, and thermal diffusivity of a rock mass. Thermal conductivity and heat capacity can appear to be artificially high during these measurements if significant quantities of heat are transferred by convective heat transfer through the rock mass and openings. This can be particularly significant near the boiling point of water because of the relatively large amount of heat per unit volume required to transform liquid water to a gas. The use of artificially high heat-capacity and thermal-conductivity values in calculations to predict repository and canister temperatures can result in actual temperatures during the operations phase that are higher than predicted. This illustrates the influence that convective heat transfer can have on the thermal properties of rock. Conversely, since the thermal properties influence temperatures, they can have an influence on convective heat transfer.

As previously discussed, convection can also influence gaseous diffusion of radionuclide chemical species, and radionuclide leakage from the repository system. It should also be mentioned that since convective heat transfer influences temperatures, which, in turn, influences thermal expansion, it also interacts, though somewhat indirectly, with thermomechanical parameters (*e.g., in situ* stress changes, displacement and deformation, induced fractures, and decrepitation and spalling).

3.1.9.1 Normal parameter range

Modeling results and measurements that give the normal range of convective heat transfer expected in the unsaturated tuff of the Topopah Springs Member are not yet available.

3.1.9.2 Is this parameter site sensitive?

Because convective heat transfer depends on a number of other parameters, as discussed in the final paragraphs of Section 3.1.9, and these other parameters are site sensitive, convective heat transfer is also site sensitive.

3.1.9.3 Expected parameter variations during normal site operations

Convective heat transfer can be expected to vary with time as temperature fields and near-field hydrology vary. Specific data on these time dependent variations are not yet available.

3.1.9.4 Parameter values that may signal trouble

In most cases, convective heat transfer, especially during the operations phase, will be beneficial, unless the heat is transferred to locations where temperatures must be kept below certain critical levels (*e.g.*, where sensitive instruments, transducers, or electronics are located). Excessive temperature rises at these locations can signal trouble, possibly from convective heat transfer. Another case that can signal trouble is conceivable if a design consideration relies on convective heat transfer, and that rate of transfer is less than expected.

Excessive convective flow might also signal trouble because of its potential influence on near-field hydrology, and its ability to act as a radionuclide transport mechanism.

3.1.9.5 What may happen if this parameter is not measured?

Thermal properties of the rock mass are critical in determining the rate of heat transfer from waste packages. Excessive convective heat transfer not properly taken into account during *in situ* measurements for site characterization can result in apparent values of rock-mass thermal conductivity and heat capacity that are artificially high. Without representative values for thermal properties and convective heat transfer; waste, canister, backfill, rock, air, and water and vapor temperatures within the repository system cannot be adequately modeled. This modeling is important to ensure that nuclear waste forms do not exceed certain maximum temperatures that will adversely affect radioactive release rates.

3.1.9.6 Measurement conditions and potential instrumentation problems

Time variations in temperature, combined with near-field variations in hydrology, can make it extremely difficult to obtain representative values for the effects of convective heat transfer in isolated volumes of the repository system. This is particularly true where heat piping takes place, because of the erratic behavior that can result from liquid-phase water supply instabilities caused by interactions between the heat piping and local hydrology. For example, condensation from heat piping can cause local changes in the degree of saturation, resulting in localized oscillations between saturated and unsaturated flow. This, in turn, can cause oscillations in the liquid-phase supply to the high temperature region of the heat pipe. Changes in near-field hydrology, such as the degree of saturation, can also cause changes in gas- and liquid-phase convective circulations within the rock formation.

3.1.10 Decrepitation and Spalling

The critical concern with rock decrepitation and spalling is their effect on the thermal properties in the very-near-field regions surrounding waste canisters. Under certain conditions, decrepitation and spalling can decrease the overall heat transfer properties near the canisters resulting in increased canister temperatures.

The following scenario illustrates the potential problem. Radiogenic heating from waste will cause thermally induced stress changes in the rock immediately surrounding the canisters. These stress changes, combined with the initial *in situ* stresses, will cause decrepitation fracturing in borehole walls where the rock strength is exceeded. This, in turn, can result in the spalling of small pieces of rock from the borehole walls into the open volumes around the canisters. Spalling will be a particular concern where borehole liners are not used, or where boreholes are not backfilled following canister emplacement. Decrepitation fractures (which may open as the stress field moves outward with thermal propagation through the rock, or as hydrous mineral phases in the tuff dehydrate), and voids between fragments of spalled rock can provide dead air spaces under dry conditions, acting as a thermal insulation. The added thermal insulation will cause an increase in canister temperature, which can result in further decrepitation and spalling. The net result is a regenerative feedback, sometimes referred to as "thermal runaway." Thermal runaway, should it occur, can conceivably cause waste forms to exceed their maximum design temperatures.

Decrepitation and spalling in saturated tuff can also affect water inflow around the canisters. Increased water inflow will most likely decrease canister temperatures. However, it may increase the potential for canister (or liner) corrosion and radionuclide release, depending on the flow rate and water chemistry.

The preceding paragraphs infer interactions that can occur between rock decrepitation and the following other critical parameters:

- thermal expansion
- initial *in situ* stress
- stress changes
- rock strength
- induced fractures
- thermal conductivity and diffusivity
- temperature
- water inflow
- canister corrosion rate
- radionuclide release

A number of other critical parameters can also interact with rock decrepitation and spalling. For example, permeability and porosity can be influenced by decrepitation. Water inflow rate in decrepitated rock will be influenced by hydraulic head or water potential. Rock modulus, Poisson's ratio, and fracture properties can also be affected by rock decrepitation. Rock mineralogy can influence strength and, consequently, the susceptibility to decrepitation.

During the site characterization phase, experiments should be conducted to determine the susceptibility of site-specific tuff to decrepitation and spalling. Laboratory tests can be made on stressed and heated samples, but *in situ* heated rock tests using canister-sized heaters in underground repository test facilities will better simulate actual repository conditions. Measurements should also be made on actual or simulated decrepitated and spalled rock to determine potential worst case thermal properties. Since rock susceptibility to decrepitation and spalling may be dependent on the amount of time at elevated temperatures, experiments during site characterization should be extended over the maximum period that the site characterization phase will allow.

Rock decrepitation and spalling will continue to be a critical parameter during the repository operations phase unless experiments during the site characterization phase show conclusively that decrepitation and spalling will not occur, or show that, if they do occur, canister temperatures will not exceed a maximum safe design value. The use of borehole liners, or the backfilling of canister storage holes can also reduce the necessity to monitor for decrepitation or spalling. There are numerous methods to monitor for decrepitation and spalling ranging from direct observations using borescopes to emplacing complex sensor systems to monitor for rock fragments in boreholes, but probably the simplest and most direct method is to monitor canister surface temperatures for sudden transients using simple temperature sensors (*e.g.*, thermocouples). Acoustic emission (AE) monitoring can also give valuable data indicating possible rock decrepitation.

3.1.10.1 Normal parameter range

Repository designs and maximum temperatures should be such that under normal operating conditions there will be negligible or no rock decrepitation or spalling.

3.1.10.2 Is this parameter site sensitive?

The susceptibility of rock to decrepitation and spalling, and the resulting thermal properties depend on hydrologic characteristics, rock mineralogy, *in situ* stress, rock strength, and rock thermal properties, all of which can vary from site to site or even within a particular repository horizon. Therefore, this parameter is site sensitive.

3.1.10.3 Expected parameter variations during normal site operations

Changes in the susceptibility of tuff to decrepitation and spalling following long periods of exposure to high temperatures have not yet been determined. There is little tabulated data on decrepitation or spalling in tuffs and the possible effects on canister temperatures. However, there is some information on this subject from experiences encountered during heated rock experiments in granite. Large-scale decrepitation and spalling occurred around a five kilowatt electrically heated HLW canister simulation after peripheral heaters were turned on during the Stripa, Sweden experiments. Canister temperatures increased 31.5°C in a period of less than 30 hours following the initial spalling. Prior to that, temperatures had been increasing steadily at about 1°C per six hour period. The first six hour period following initial spalling showed a temperature increase of approximately 16°C (Chan *et al.*, 1980, Appendix D microfiche; E.P. Binnall, Stripa Experiment Field Notes, February 7, 1979).

3.1.10.4 Parameter values that may signal trouble

A sudden increase in canister temperature can indicate large-scale rock spalling around a canister, or unexpectedly high canister temperatures may be a result of slower rock decrepitation. Sudden increases in water inflow, probably accompanied by a sudden decrease of canister temperature, can also indicate rock decrepitation and/or more extensive induced fracturing in a saturated tuff environment.

Heavy spalling can make it difficult to backfill around canisters, and difficult to remove canisters if they should need to be retrieved.

3.1.10.5 What may happen if this parameter is not measured?

The susceptibility of site specific tuff to decrepitation and spalling, and the thermal properties of the decrepitated and spalled tuff are among the parameters that must be considered in the repository, canister, and waste form design to ensure that thermal runaway will not occur, and that the waste form and other materials will not exceed design temperatures, or be exposed to excessive water flow.

3.1.10.6 Measurement conditions and potential problems

The nonhomogeneous characteristics of tuff make it difficult to determine characteristic and worst case susceptibility to decrepitation and spalling without a significant number of tests throughout the repository during the site characterization phase. The same equipment and locations used to determine *in situ* thermal conductivity, heat capacity, and diffusivity (Section 3.1.8) can also serve to test for decrepitation and spalling susceptibility by increasing heater temperatures and/or extending the test periods.

Any monitoring for decrepitation and spalling near waste canisters during the operations phase will require using procedures and precautions established for work in the vicinity of radioactive material.

3.1.11 Canister Movement

Canister movement will probably not be of any significant concern for a repository horizon located above the water table in the Topopah Springs Member, assuming that reasonable engineering precautions are taken. The principal concern regarding potential canister movement will arise if a repository horizon is selected at an elevation well below the water table, where hydrostatic pressures are large. In general, canister movement in storage boreholes can be caused by forces acting directly on canisters or by forces transmitted through backfill material. Driving forces can originate from a number of sources, including:

- hydrostatic pressure
- steam
- expansion of clay in backfill mixtures due to hydration
- rock deformation
- rock failure

Massive rock failure can cause canister movement in open boreholes. However, for repository horizons well below the water table where hydrostatic pressures are significantly large, it is more likely that canisters will be exposed to driving forces that can cause significant movement after the volumes around the canisters become tightly sealed with hydrated backfill. Most of the backfill mixtures under consideration contain dehydrated clay that expands and improves sealing characteristics when wetted (*e.g.*, bentonite).

Assuming a tightly sealed backfill scenario in a repository located well below the water table, hydraulic and steam pressure are the two most likely candidates capable of creating driving forces with sufficient volumes to cause significant canister movements. Water intrusion into a storage borehole, vertical or horizontal, with backfill surrounding the canisters can initiate a series of events that can ultimately cause movement of a single canister or a string of canisters. First, water inflow, say at a single fracture intersecting the borehole, can cause expansion of clay in the backfill, enhancing the seal around the canisters. With a tight enough seal, hydrostatic pressure can create a pressure gradient across the borehole, or more likely, down its length. Expansion of the clay itself can also act as a pressure source. However, the pressure source with the largest volumetric capacity will probably be steam generated from water heated by the waste canisters; that is, until water inflow causes pressure that exceeds the vapor pressure of the heated water. If the vapor pressure is exceeded, hydraulic pressure, which can ultimately reach the hydrostatic pressure at the repository depth, will be the dominant pressure

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source. The magnitude of the pressure gradient will depend on the ability of pressures to equilibrate through and around the backfill material, the amount of backfill compression and extrusion that takes place, and the extent of pressure relief paths (either intrinsic to the rock structure or designed into the repository system). However, pressure relief paths can also be potential paths for radionuclide escape. Canister movement will occur when the forces across the pressure gradient exceed the forces holding the canister(s) in place.

To illustrate the potential problem, assume that a fracture opens in the wall of a backfilled, horizontal storage borehole, so that one end of a 0.457 m (18 in.) diameter canister, midway in a string of end-to-end canisters, becomes subjected to water inflow. Also assume that pressure equilibrates very slowly through the backfill along the borehole length, resulting in the full pressure gradient appearing along the canister string in such a way that the opposing pressure on the canister string remains close to one atmosphere; and assume that the canister surface is at a maximum temperature of 300°C. Since the vapor pressure of water at 300°C is 8.59 MPa (1246 psi) (CRC Handbook of Chemistry and Physics, 1972), steam can be generated with pressures up to 8.59 MPa (1246 psi). This translates into a potential driving force of up to 1.41×10^6 N (0.317×10^6 lbs.) on the cross-sectional area at one end of the canister string.

If hydrostatic pressure at the canister depth is greater than the vapor pressure of the heated water, water inflow can continue in liquid state until pressure behind the canister end reaches hydrostatic pressure, assuming that nothing happens to relieve the pressure buildup. Canister movement is one mechanism by which these very large driving forces can be relieved.

Rock deformation (thermomechanical, etc.) and rock failure, particularly in unlined boreholes tightly sealed by rehydrated backfill, can create driving forces on canisters considerably greater than potential forces from water inflow. However, even though rock deformation can cause extremely high pressures, the volumetric displacement should be insufficient to cause any significant canister movement. Pressures created by massive rock failures can approach lithostatic pressures, or pressures equivalent to the maximum horizontal stress fields. Even though a massive rock failure can cause significant canister movement, the design of the repository should be such that the probability of this type of failure in and around a canister borehole will be extremely low.

Canister movement can interact with the following other critical parameters:

- water inflow rate
- permeability
- water potential or hydraulic head
- fracture properties
- *in situ* stress and stress changes
- displacement and deformation
- rock modulus and Poisson's ratio
- thermal expansion
- induced fractures
- thermal conductivity, heat capacity, and diffusivity
- rock strength
- seal and backfill leakage
- decrepitation and spalling
- radionuclide release

Most of the ways by which these interactions can occur are apparent from the preceding discussions in this section.

Monitoring and measuring canister movement is considered as being critical only during the site operations phase when radioactive canisters are in place, and only for repository horizons located below the water table. The most likely time for canister movement will be during the period after hydration of backfill around the canister, and before pressures have had adequate time to equilibrate throughout the backfill volume. Knowledge of canister movement will become particularly important if retrieval should become necessary. This is also true if it should become necessary to open a closed repository or repository section for canister retrieval during the closure phase. Opening a repository section after pressures have equilibrated can cause large force imbalances that, in turn, can have the potential to cause significant movements of backfill material and canisters. Even though small movements can relieve hydraulic forces, reducing the pressure on super-heated water can cause it to flash into steam, providing high-volume force potentials at significant pressures, capable of causing large movements of backfill and canisters. Even taking this into consideration, with present technology, the potential benefits do not appear to outweigh the possible problems that might result from attempts to directly monitor for canister movement after initiating the closure phase.

In situ testing, using heated canister simulations set up for other critical parameter measurements during the site characterization phase, should also provide data on the sensitivity of canisters to movement from pressure gradient buildup. However, in itself, canister movement is not considered a critical parameter during the site characterization phase.

3.1.11.1 Normal parameter range

The repository and canister storage design should be such that significant canister movement will not take place under normal operating conditions.

3.1.11.2 Is this parameter site sensitive?

This parameter depends first on whether the repository horizon is located above or below the water table. The possible forces that can act on canisters to cause their movement are dependent on permeability, hydrostatic pressure, lithostatic pressure, *in situ* stress, fracture properties, and rock strength, all of which can vary from one site to another. Therefore, the potential for canister movement is site (and design) sensitive.

3.1.11.3 Expected parameter variations during normal site operation

Forces acting on canisters that may cause their movement will vary as repository conditions vary with time. For example, in saturated regions fractures may open, changing water inflow rates behind backfilled canisters as thermomechanical stresses move outward through the rock. However, quantitative estimates of expected variations in the probability for significant canister movements are not available at this time.

3.1.11.4 Parameter values that may signal trouble

Canister movements that may signal trouble will probably be on the order of centimeters or greater; at least large enough to make retrieval difficult should it become necessary, or large enough to move a canister from a protected and shielded location in its storage borehole.

3.1.11.5 What may happen if this parameter is not measured?

In a questionable environment, canister movement may become so great before corrective action can be taken that retrieval could become difficult, or engineered barrier protection from radioactive release could become significantly reduced.

3.1.11.6 Measurement conditions and potential problems

Installing instrumentation to monitor for canister movement without compromising the backfill seal might be the most difficult problem. Direct measurement instrumentation may need to be in close proximity to radioactive material, making it difficult to check or service the instrumentation.

3.2 Geologic Parameters

Geological parameters fall into two categories: those that can be measured directly, and those that have no instrumentation for their direct measurement, but require application of one or more geophysical techniques for their characterization and continued monitoring.

The former category, described first in this section, includes direct, or nearly direct measurement of crustal deformation, naturally occurring radionuclides, and seismicity. The latter category, described subsequently, includes lithology, faulting, folding, erosion rate, igneous activity, and the presence of water, mineral, and petroleum resources. With the exception of the resources (whose presence would be discerned by a literature search), these parameters are indirectly measurable by a combination of geophysical techniques employing surface, borehole, and airborne surveys. For example, the depth, lateral extent, and thickness of lithologic units might be discerned by high-resolution active seismic surveys and to a lesser degree by electrical and/or electromagnetic measurements. These types of measurements would be employed extensively in surveys conducted during the site characterization phase, in conjunction with measurements in widely spaced drill holes and analyses of samples from these holes. After a shaft has been sunk and significant excavation for the initial test facility started, direct observation of most geologic parameters will be afforded by the underground workings. Horizontal, continuously cored holes, drilled from these workings would then provide sets of core samples for geological observations as well as material for preliminary laboratory measurements of physical

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and hydrological properties of the host rock in the candidate repository. The horizontal holes might also provide locations for specific active seismic and/or electromagnetic geophysical measurements.

3.2.1 Crustal Deformation

Long-term crustal deformation, including uplift, lateral and vertical offsets along faults, subsidence, and crustal lengthening or shortening, can perturb groundwater flow paths and surface mass wasting processes, conceivably either improving or diminishing the ability of a site to inhibit migration of radionuclides. A localized uplift may occur in response to the thermal regime introduced by the presence of the radioactive waste. To assess these effects at a site, long-term monitoring of crustal deformation is required. Such monitoring depends on establishment of geodetic measurement networks spanning the site region. The networks include leveling transects for vertical control, and length-measurement segments to detect horizontal components of crustal movement. The networks should be established early enough in the site characterization phase to provide a set of baseline data, against which results of subsequent surveys will be compared. The extent of the networks should be broad enough to include points outside the site area that can serve as fixed benchmarks. The tectonic setting of the Yucca Mountain site at the Nevada Test Site (NTS) is considered in this context.

3.2.1.1 Normal parameter range

Considerable crustal shortening occurred in what is now the southern Basin and Range geomorphic province over the period from ~360 to 75 million years ago. This is manifested by thrust faults in the pre-Tertiary rocks of the region (Smith *et al.*, 1981). Basin- and range-style faulting, exemplified by numerous normal faults, commenced 18 to 13 million years ago (Carr, 1974; Smith *et al.*, 1981) and continues today. As described in Section 3.2.5 (Faulting), vertical displacements in the region vary from hundreds to tens of meters, and in the site area from tens of meters to a few meters (DOE, 1984, Section 3.2.2).

3.2.1.2 Is this parameter site sensitive?

Crustal deformation occurring in the Yucca Mountain block over the operating life and post-closure periods of the repository is expected to take place principally in the form of vertical movement, and to a lesser extent lateral movement, on the normal faults that transect the site area. Tilting of blocks between the faults would likely occur in response to these fault movements. Therefore, limiting the extent of critical portions of the underground workings so that they are not crossed by these faults should obviate sharp vertical and lateral offsets associated with future movements on the faults.

3.2.1.3 Rationale for continued measurements

Vertical- and horizontal-control geodetic surveys over established networks are required periodically throughout the site operating phase, closure, and beyond. Localized uplift, that might occur in response to the thermal effects from the waste, can only be assessed by precise vertical control based on long-term observations.

3.2.1.4 Expected parameter variations during normal site operations

Over the operating (pre-closure) period of the repository, deformation is expected to be negligible, as evidenced by the absence of deformation over the past several thousand years.

3.2.2 Naturally Occurring Radionuclides

The gamma radiation environment, upon which the effects of the introduction of radioactive waste will be superimposed, depends on the abundances of the naturally occurring elements: uranium, thorium, their decay products, and potassium. A survey of the location and abundance of these elements in the rock-matrix, fracture-filling minerals, and groundwater establishes the natural environmental radioactivity baseline, and also aids in the determination of the age and origin of groundwater, thus assisting in evaluation of the hydrologic suitability of a candidate site. A knowledge of radioelement location and abundance will also help to determine the likely path of radionuclide transport into and through the hydrologic system of the rock mass encompassing the repository.

The distribution and abundance of U and Th in the rock matrix and fracture-filling minerals provide indications of the mobility of these elements in and away from a repository environment. For example, differences observed between concentrations of U and Th in the rock matrix and in fracture- and vug-filling minerals indicate the ability of these minerals to adsorb radioelements from water circulating through

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these openings. An investigation of the state of secular equilibrium in the U and Th decay series in fracture-filling minerals reveals the varying mobility of members of the mineral assemblage. Monitoring of the U-series daughter, ^{222}Rn, in the atmosphere of the underground workings is necessary to establish the initial environmental radiation baseline and to detect subsequent increases that might result from water inflows, rock deformation, and heating of the rock (Nelson *et al.*, 1980).

A knowledge of contents of uranium isotopes in the groundwater can be used to estimate the age of the water, an important parameter in assessing the degree of isolation of the hydrologic system encompassing the repository. Corroborative age information may be obtained from measurements of the He content of the water, combined with contents of U and Th in the rock. Age dating of groundwater is discussed in Section 3.4.2.

The contents of radioelements in the rock are readily determined by laboratory gamma spectrometry, substantiated by delayed neutron and/or neutron activation analyses. With appropriate calibrations provided by laboratory analyses, it has been demonstrated that reliable concentration values can be obtained by measurements in underground workings by a portable gamma spectrometer (Wollenberg *et al.*, 1980). The gamma-ray exposure rates due to the presence of U, Th, and K in the rock can then be calculated by applying conversion factors, adjusted for the 4π geometry provided by the workings.

3.2.2.1 Normal parameter range

The distributions and abundances of U, Th, and K strongly depend on rock type, and felsic ash-flow tuffs have relatively high concentrations compared to most igneous rocks. However, as Rosholt and Noble (1969) point out, devitrification of glassy groundmass material in tuff may result in mobilization of U and its removal by groundwater. Crystallized ash flow tuffs may then have substantially lower U concentrations than their non-crystallized counterparts.

Means and standard deviations of radioelement concentrations of 124 data-base entries for rhyolite and rhyodacite (rock types that encompass the compositional range of ash-flow tuff) are:

U(ppm)	Th(ppm)	K(%)
6 ± 4	22 ± 15	3.7 ± 2.6

(Wollenberg and Smith, 1985). These values are roughly three times the concentrations in Columbia River Basalt.

Data on uranium concentrations of groundwater in felsic tuffaceous terranes are scarce. Some cold springs in northern Nevada, recharged from a rhyolitic tuffaceous highland have U concentrations ranging from 0.1 to 3.5 μg/L (Wollenberg *et al.*, 1977). It is expected that in some tuffs, groundwater U concentrations may reach 10 μg/L.

3.2.2.2 Expected parameter variations during normal site operation

Variations detected in the natural radionuclide contents of groundwater, as with variations in other chemical constituents, would indicate changes in the hydrologic regime. Addition of chemical components of one aquifer system into another system would indicate hydrologic connection, perhaps along vertical fractures or along pathways caused by excavation and operation of the repository. For these reasons, chemical signatures of the aquifer systems present in a tuff sequence must be well established and periodically monitored.

3.2.2.3 Rationale for measurements

Investigations of the distributions and abundances of naturally occurring radioelements in the rock and groundwater, besides furnishing the natural radioactivity baseline, also would help reveal the sorptive capabilities of fracture-filling minerals, the mobility of members of the U and Th decay series in the groundwater system, and would contribute to the determination of the age and origin of the water; important factors in the evaluation of site suitability.

3.2.3 Seismicity

The effect of local and regional seismicity on underground workings involves considerations similar to those for surface facilities: the earthquake magnitudes, epicentral distance from the repository, regional geologic setting, and the nature of the materials encompassing the repository. These all influence the accelerations experienced and the duration of shaking at a given site, which in turn control the earthquake intensity at that site.

An assessment of earthquake damage to underground facilities by Pratt *et al.* (1978) suggests that the deeper the underground workings, the less their response to a given earthquake, compared to surface conditions. This is largely attributed to attenuation of the high frequency ground motions with depth below the ground surface. Vertically oriented workings, such as shafts and wells, are less prone to damage than are horizontal workings. The primary concern then, aside from the obvious one of not locating the site astride an active fault, is shaking which might disrupt support facilities on the surface and might damage the shafts. However, surface structures are very short-lived compared to the repository. The effects of earthquakes on these structures are of principal concern during the periods of repository operations and retrievability rather than during the period of long-term isolation.

3.2.3.1 Normal parameter range

Three large earthquakes have occurred in the NTS region in recorded history. The largest was the Owens Valley quake of 1872 at a distance of ~150 km to the west of Yucca Mountain. Another earthquake, with a magnitude of ~6, occurred in 1908 approximately 110 km southwest of Yucca Mountain, and one in 1966 of about the same magnitude was located 210 km to the northeast. Within 10 km of Yucca Mountain, seven quakes were recorded between August, 1978 and the end of 1983; the largest magnitudes were ~2 (DOE, 1984, Section 3.2.3). Prior to 1978, at least two quakes in this area had magnitudes of ~3.5. The maximum magnitude earthquake expected on the potentially active fault considered to present the greatest hazard to the Yucca Mountain site, is calculated to be of magnitude 6.8 (DOE, 1984, Section 3.2.3). The peak surface acceleration associated with this quake is calculated to be ~0.4g.

3.2.3.2 Is this parameter site sensitive?

The seismic response of sites in the southern Basin and Range province depends to a great extent on their structural setting: specifically the orientation and spacing of the normal faults, such as those bounding the Yucca Mountain site.

3.2.3.3 Expected parameter variations during normal site operation

As just indicated, magnitudes can range from those of microearthquakes to nearly 7. Probabilistic calculations indicate that the aforementioned maximum surface acceleration of ~0.4g has a return period of the order of 900 to 30,000 years (DOE, 1984, Section 3.2.3).

3.2.3.4 Rationale for continued measurements

Seismic monitoring networks should continue to be operated to detect any significant variations from the zonations, recurrence rates, focal mechanisms, and magnitudes observed to date. On the basis of these observations, and depending on the stage of operations, design of surface and underground waste handling facilities could be confirmed or modified.

3.2.4 Lithologic Parameters

A principal concern in evaluating a repository site in a bedded rock is the homogeneity of the candidate horizon over a lateral extent sufficient to encompass the repository and its buffer zone. In tuff, the "horizon" may comprise a specific cooling unit, or a part of that unit. Homogeneity implies that the candidate horizon has a vertical extent sufficient to contain the repository excavations (hydrostratigraphic homogeneity is discussed in Section 3.3.1). Lateral homogeneity must not only apply to the gross thickness and structual integrity of a candidate rock unit, but also to its lithologic uniformity. This in turn implies that the rock's chemical and mineralogical compositions are relatively uniform over a given area. Compositional uniformity can best be assessed by visual observation and recording of drill core and the rock exposures afforded by the walls, roof, and floor of the underground workings.

It is pointed out in Sections 3.1.2 and 3.3.2 that careful visual observation and recording of fracture spacing, orientation, and aperture are necessary to properly characterize the physical as well as hydrologic behavior of the candidate rock mass, to predict its response to excavation, the introduction of radioactive waste, and the ability of the rock mass to ultimately contain the waste. In the case of tuff, the size and spacing of lithophysae are also important considerations. Careful observation and recording of the mineralogy of material that fills the fractures and lithophysae must also be undertaken. Such observations would commence with the initial excavation at the bottom of the first shaft, and would continue through site operations as new vertical and horizontal openings were developed. Determinations of the mineralogy and chemical composition of rock-matrix and fracture- and lithophysae-filling material would disclose the presence and abundance of zeolite minerals that could adsorb radionuclides from the groundwater. This subject is discussed in detail in Section 3.4.3, Sorptive Capacity of Formation Rock.

3.2.5 Faulting

The presence and magnitude of most of the faults transecting the region encompassing a repository location would be detected in the early stages of site investigations by geologic mapping and geophysical surveys. Subsequent observations and drilling from underground workings might disclose smaller offsets not discernible from the surface. In the Yucca Mountain area some of the faults are attributed to collapse of the Timber Mountain caldera (11 to 12 million years ago) and some to the more regional basin and range faulting (DOE, 1984, Section 3.2.2). These latter faults trend northward, are of high angle, and adjacent blocks are downdropped chiefly to the west. Vertical displacements vary from tens to hundreds of meters, and within the primary site area, from a few to 20 m (DOE, 1984, Section 3.2.2). A few fault scarps, of the order of a meter in height, occur in Quaternary alluvium within 20 km of the Yucca Mountain site (DOE, 1984, Section 3.2.2). Dating of materials from trenches dug across these scarps produced no strong evidence that movement on these scarps has occurred within the last 40,000 years (DOE, 1984, Section 3.2.2).

3.2.6 Folding

As with faulting, major folds can be detected by surface mapping and geophysical surveys. Detailed expressions of folding can be disclosed from surface and borehole geophysical data. Folding is also indicated by the topography of the top of tuff units from drill hole intersections. Reoccupation of the aforementioned leveling and trilateration networks to monitor crustal deformation would also serve to monitor any ongoing development of folds.

3.2.7 Erosion Rate

The principal concern here is incisement of the site by the effects of erosion. This could be caused by two factors: short-term single or repeated erosion of the site by catastropic flooding, and erosive incision of the rock encompassing the respository in response to tectonic uplift and/or faulting. USGS investigations indicate that the mean stream incision rate is 5×10^{-5} m/yr in the vicinity of Yucca Mountain (DOE, 1984, Section 6.3.1.5.3). In the latter case, monitoring of uplift rates will indicate the propensity for erosion.

3.2.8 Water, Mineral, and Petroleum Resources

An assessment of the potential water, mineral, and petroleum resources of a site region and their valuation requires an extensive literature search as well as communication with existing and potential operators in the region. Instrumentation would not be required in this activity.

3.2.9 Potential Igneous Activity

The propensity for igneous activity to occur in a site region during the lifetime of a repository can best be assessed by investigating the recurrence rates of volcanic and intrusive episodes. Such rates can be determined from historical records and rock age dating. The youngest volcanic manifestations near Yucca Mountain are basaltic emanations (within 8 to 15 km) whose ages range from 230 thousand to 3.7 million years (DOE, 1984, Section 6.3.1.7.4).

3.3 Hydrologic Parameters

Yucca Mountain has many favorable aspects as a potential site for a nuclear waste repository, including: an extensive unsaturated zone, low rainfall and infiltration rates, and high sorptive capacity of the tuffaceous units. Nevertheless, characterizing the site, and monitoring the response of the rock mass and the hydrologic system to the operation of a waste repository, presents many challenging problems.

The difficulties arise because hydrogeologic systems such as that at Yucca Mountain were of little practical interest until now. Consequently, methodologies for measuring the physical properties of the rocks, and determining the natural state of the system (*e.g.*, infiltration rates, the role of faults and fractures in the hydrologic system, and vapor flux) are lacking. Techniques used for this purpose are borrowed from soil scientists, petroleum engineers, and groundwater hydrologists. As such, many of the physical concepts (*e.g.*, relative permeability, and saturation characteristic curves) and empirical relations (*e.g.*, saturation and relative permeability) are being used outside the range for which they were originally validated. Considerable effort must be devoted to validating physical concepts, developing appropriate empirical correlations among parameters, and developing instruments and measurement techniques that are appropriate for measuring the critical parameters in unsaturated, fractured-porous rock.

The most likely means by which radionuclides will travel to the accessible environment is through the groundwater system. Water coming in contact with the canisters will leach the radionuclides from the waste form, carry the soluble radionuclides down-gradient, and eventually discharge them in regional or local groundwater sinks. Along the way, some of the radionuclides will be adsorbed onto the rock surfaces, diffuse into the rock matrix, and decay into other species, thereby retarding the rate at which these products will enter the accessible environment. At the same time, volatile radionuclides will diffuse under both temperature and concentration gradients through the air-filled pore spaces in the rock. Both of these release mechanisms must be considered to accurately predict the rate, quantity, and distribution of radionuclides entering the accessible environment.

Extensive laboratory and field experiments are required to provide the basic data on fluid flow and chemical transport in the tuffs at Yucca Mountain. Current practices for evaluating fluid flow in partially saturated rocks are not adequate for characterizing the flow regime at Yucca Mountain, nor are they adequate for the purpose of predicting the influence of a waste-repository located in the partially saturated zone. Major uncertainties result primarily from two sources. First, the appropriate scales (size of rock sample) for measuring and modeling the transport properties of the rock have not been identified. Second, the role that faults, fractures, and the rock matrix play in the overall fluid and chemical transport processes at work at Yucca Mountain are uncertain. Until these issues are resolved, it will be difficult to choose conservative values for the parameters used to calculate the rate at which radionuclides are released to the accessible environment.

3.3.1 Hydrostratigraphic Units

A hydrostratigraphic unit is defined as a rock unit that behaves in a hydrologically uniform manner. Within a hydrostratigraphic unit, each physical property such as directional permeability, porosity, and compressibility remains the same. Depending on the scale appropriate to the region of interest, a hydrostratigraphic unit may encompass an entire ash-flow unit, a lithophysal zone within an ash-flow, the nonwelded unit within the flow, a fractured zone within a unit, or the contact between two ash-flow units. Close to the underground repository, highly detailed definition of hydrostratigraphic units is required. For instance, individual fractures or lithophysal zones must be characterized. On the other hand, far away from the repository, less detailed definition is required. Accurate characterization and identification of the hydrostratigraphic units throughout the groundwater system is required in order to locate the permeable pathways along which soluble and volatile radionuclides will migrate to the accessible environment. Numerical modeling to predict the hydrologic impact of locating a repository at Yucca Mountain, also requires adequate definition of hydrostratigraphic units.

Hydrostratigraphic units are identified by correlating lithologic, mineralogic, hydrologic, geochemical, and perhaps, geomechanical data among boreholes and excavations. Correlatable rock units with the same hydrologic properties are defined as hydrostratigraphic units. To adequately define a hydrostratigraphic unit, all of the physical parameters must be determined. For instance, it is not sufficient to infer that two correlatable lithologic units have the same permeability. Rock permeability can vary by orders of magnitude within a single lithologic unit.

The measurements required to identify and characterize hydrostratigraphic units cover the spectrum of lithologic, geochemical, geophysical, and hydrologic test techniques, including: geologic mapping, borehole logging, analysis of pore fluids, and pump tests. The techniques and measurements are discussed under their respective disciplines and therefore, are not repeated here.

3.3.1.1 Normal range

Not applicable.

3.3.1.2 Is this parameter site sensitive?

This parameter is highly site specific.

3.3.1.3 Expected parameter variations during normal site operation

Uncertain, although construction and operation of a repository may result in the creation of new hydrostratigraphic units in the near-repository rock.

3.3.1.4 Parameter values that may signal trouble

None.

3.3.1.5 Role during each repository phase

Identification and characterization of the hydrostratigraphic units throughout the groundwater basin will take place primarily during the site characterization phase. However, definition of the near repository units will continue during site construction. By the end of the site construction phase, it is assumed that the hydrostratigraphic units will have been adequately characterized, and will thereafter remain the same.

3.3.1.6 Measurement conditions and potential instrumentation problems

The main uncertainties with identifying and characterizing the hydrostratigraphic units in the Yucca Mountain area result from: 1) the highly heterogeneous nature of the tuffs, and 2) the difficulty of measuring the hydrologic and transport characteristics in the unsaturated zone. For a more detailed discussion, see descriptions of the individual parameters under their respective disciplines.

3.3.1.7 What may happen if this parameter is not measured?

Without adequate identification of the hydrostratigraphic units in the vicinity of the proposed repository location and the surrounding groundwater system, the site can not be considered for the isolation of high-level waste (HLW).

3.3.2 Permeability (Fracture and Matrix)

The saturated permeability of a rock is a measure of its intrinsic ability to conduct fluid; the higher the permeability, the more quickly water will travel through it. In the following discussion, the term permeability refers to the permeability of a fully saturated rock. In a partially saturated medium, the actual fluid velocities are a function of both the intrinsic permeability of the rock and the relative permeability to a given fluid (which is a function of its degree of saturation). Refer to Section 3.3.3 for a discussion of relative permeability, and to Section 3.3.4 for a discussion of the degree of saturation. Gaseous diffusion is discussed in the Appendix.

In tuff, the permeability results from both the fractures and pore spaces in the rock matrix. Usually, the fracture permeability is greater than that of the matrix. In general, it is a directional quantity and must be described in terms of a tensor. However, it is customary to determine only two of its components, the horizontal and vertical permeability. For fractured rocks, the validity of formulating fluid flow and chemical transport equations in terms of the permeability tensor depends on the ability to define a suitable "representative elementary volume" over which an average permeability can be measured. Long (1983) established the theoretical framework for determining when a randomly fractured rock can be treated as an equivalent porous medium. When the fractured rock can not be treated as an equivalent porous medium, the fluid flow and chemical transport equations must be written in terms of discrete and identifiable flow channels within the rock. For practical applications, the complexity introduced by this second possibility is beyond the ability of modern day fracture mapping techniques and computing capabilities.

The rate at which a fluid travels through a permeable rock is related to the permeability by Darcy's law; that is:

$$v = \frac{-k}{\mu}\left(\nabla p + \rho g \nabla z\right) ,$$

where k is the permeability, μ is the fluid viscosity, p is the fluid pressure, ρ is the fluid density, g is the acceleration due to gravity, z is the elevation above a given datum, and v is the Darcy velocity of the fluid. Insofar as the rate at which fluid flows through a rock matrix is proportional to the permeability, the rock permeability interacts with almost all of the critical hydrologic parameters: fluid velocity, water infiltration rate, groundwater recharge and discharge (location and rate), age of water, and water inflow rate. Because predictions of the future behavior of these parameters and the interpretation of current conditions are calculated from the permeability, errors in the calculated permeability are directly transferred to these parameters. For instance, an uncertainty of a factor of two in the permeability of the rock results in an uncertainty of a factor of two in the estimated water infiltration rate and the calculated transit time to the accessible environment.

In the groundwater literature, it is common to describe the saturated fluid flow and chemical transport equations in terms of hydraulic conductivity, rather than permeability. The hydraulic conductivity (K) is related to the permeability (k) by

$$K = \frac{k\rho g}{\mu} \ ,$$

where ρ is the fluid density, g the acceleration due to gravity, and μ is the fluid viscosity. Under nonisothermal conditions, the hydraulic conductivity can change by an order of magnitude because both the fluid viscosity and density are temperature dependent. When hydrologic tests are conducted under nonisothermal conditions, the temperature to which the measurements correspond must be determined (Benson and Bodvarsson, 1982; Benson, 1984). If fluid properties corresponding to the incorrect temperature are used, the calculated permeability can be in error by as much as an order of magnitude. To avoid confusion between actual changes in the rock properties and changes in the fluid properties resulting from nonisothermal conditions, it is appropriate to report the test results in terms of the true rock permeability (k) and to make note of the temperature at which the test was conducted.

3.3.2.1 Normal parameter range

The permeability of tuff is extremely site specific and highly variable. Saturated matrix permeabilities of 1.5×10^{-19} to 1.9×10^{-18} m^2 have been reported for the representative samples of the densely welded tuff; saturated matrix permeabilities for representative samples of the vitric, non-welded tuff range from 2.7×10^{-16} to 4.0×10^{-14}; and the saturated matrix permeability of a representative sample of the zeolitized, nonwelded tuff is 2.0×10^{-18} (Peters *et al.*, 1984).

3.3.2.2 Is this parameter site sensitive?

This parameter is highly site specific.

3.3.2.3 Expected parameter variation during normal site operation

Changes in permeability resulting from constructing and operating a repository at Yucca Mountain will be limited to the near-repository region. These changes, which may increase or decrease the permeability, result from stress redistribution around the underground openings, fracturing of the rock at the walls of the underground openings, and hydrothermal alteration. Changes in the near-repository rock permeability are not expected to lessen significantly the ability of the repository to isolate the HLW (Sinnock *et al.*, 1984).

3.3.2.4 Parameter values that may signal trouble

These values are uncertain.

3.3.2.5 Role during each repository phase

During site characterization, *in situ* tests need to be conducted in boreholes and excavated chambers in order to measure the bulk horizontal and vertical permeability of rock units throughout the hydrostratigraphic units above, in, and below the repository horizon. Tests will also be conducted throughout the groundwater basin to fully characterize all units that potentially affect the ability of the site to isolate HLW. Laboratory tests will be conducted in order to measure the matrix permeability of rock cores from each of the hydrostratigraphic units.

During site construction, *in situ* tests will be continued in order to develop a more detailed description of the near-repository rock, detect excavation-induced permeability changes, and confirm the reliability of prior measurements. Laboratory tests to measure the matrix permeability of the newly excavated rock will continue until all hydrostratigraphic units in the near-repository rock are fully characterized.

3.3.2.6 Measurement conditions and potential instrumentation problems

The permeability of a rock mass is usually inferred from the measurement of fluid flow rate while a controlled hydraulic gradient is imposed, or vice versa. In partially saturated rock, conventional techniques are complicated by relative permeability effects (see Section 3.3.3), air entrapment, capillary flow, changes in fluid saturation (see Section 3.3.4), lack of gravitational equilibrium and sub-atmospheric pore pressures (see Section 3.3.7). Novel test techniques are being developed such as gas injection tests, however, these techniques are still developmental and cannot be applied with great confidence at this time (Montazer, 1982). Due to a lack of well established techniques for measuring the permeability of partially-saturated fractured-porous rocks, accurate measurement of bulk formation permeability will be difficult in the partially saturated zone. Laboratory tests are reasonably accurate for determining matrix permeability. However, the results are strongly biased by sample-size and heterogeneity within the rock sample (Peters *et al.*, 1984). Large discrepancies have been observed between laboratory and field measured permeabilities, especially in partially saturated systems (Olson and Daniel, 1981).

Recent research has shown that unlike fully-saturated systems, in which liquid flows mostly through high permeability fractures; liquid flows preferentially through the rock matrix in a partially saturated medium (Wang and Narasimhan, 1984; Montazer, 1982). Therefore, the uncertainty associated with calculating the bulk permeability (fractures and matrix) in the unsaturated zone may not be as critical as it is in a fully saturated rock. Nevertheless, evaluation of the transport of volatile radionuclides in the gas phase still requires accurate assessment of the fracture permeability. In addition, the near-repository hydrologic and thermal response to canister emplacement is strongly influenced by the presence of high-permeability fractures (Pruess *et al.*, 1984).

3.3.2.7 What may happen if this parameter is not measured?

It is not possible to predict the rate at which radionuclides are released to the accessible environment without accurate measurement of the permeability in the saturated and unsaturated zones. Therefore, permeability measurements are required.

3.3.3 Relative Permeability

When more than one fluid or fluid phase exists within the pore space of a rock, the rate at which a given fluid flows through the rock is influenced by the presence of the other(s). When two fluids are present, the second fluid reduces the cross-sectional flow area and increases the length of the flow path (tortuosity) of the other fluid, thereby, decreasing the rate that a given fluid can flow through the rock. At low saturations, especially for the wetting-fluid (the fluid that preferentially fills the smallest pore spaces), the effective permeability of the rock can be reduced by several orders of magnitude.

The factor which accounts for this phenomenon is called the relative permeability. It ranges from one (for a fully saturated rock) to zero, depending on the degree of saturation. For partially saturated flow, the Darcy flow equation is modified to include this effect as follows:

$$\boldsymbol{v}_w = \frac{-kk_{rw}(s_w)}{\mu_w}\left(\nabla\phi_p + \rho_w g\nabla z\right)$$

for the liquid, and

$$\boldsymbol{v}_g = \frac{-kk_{rg}(s_g)}{\mu_g}\left(\nabla p_g + \rho_g g\nabla z\right)$$

for the gas phase (air and water vapor); where $\boldsymbol{v}_w$ and $\boldsymbol{v}_g$ are the Darcy velocities of the water and gas at saturations of s_w and s_g, k is the absolute permeability, k_{rw} and k_{rg} are the relative permeabilities of the water and gas, μ_w and μ_g are the viscosities of the water and gas, $\nabla\phi_p$ and ∇p_g are the pressure gradients in the water and gas phases, ρ_w and ρ_g are the densities of the water and gas, g is the acceleration due to gravity, and z is the elevation.

Insofar as the rate at which fluid flow through the subsurface is proportional to the effective permeability (kk_r), the relative permeability interacts with most of the critical parameters for the partially saturated zone, including: liquid and gas velocities, water infiltration rate, age of water, and water inflow rate. For a more complete discussion of the interaction between permeability and the other critical parameters, see Section 3.3.2, Permeability (Fracture and Matrix).

Relative permeabilities are usually measured in the laboratory on core-sized rock samples. The relative permeability-characteristic curves, which establish the relation between the relative permeability and pressure head, are measured for both the liquid and gas. The relation between saturation and relative permeability is determined by correlating the saturation-characteristic curve (saturation *vs* pressure head) to the relative permeability-characteristic curve. Relative permeabilities are strongly hysteretic, that is, they depend on whether the rock is in the process of drying or wetting. In order to fully characterize the rock, measurements during both wetting and drying are required.

In the soil sciences, relative permeability is often calculated from the pore size distribution of a soil sample (Mualem, 1976; Van Genuchten, 1978; Elzeftawy and Cartwright, 1981). This approach is currently being used to estimate the liquid-phase relative-permeabilities of the tuffaceous rocks at Yucca Mountain (Peters *et al.*, 1984; and Sinnock *et al.*, 1984). The validity of this technique for calculating hard-rock relative permeabilities has not been demonstrated (Evans, 1983).

3.3.3.1 Normal parameter range

Relative permeabilities range from zero to one. For homogeneous rocks, typical functional forms of the air-water or oil-water relative permeability curves are often expressed in terms of

$$k_{rw} = \left[\frac{s_w - s_0}{1 - s_0}\right]^3$$

for the liquid component, and

$$k_{rg} = \left[\frac{s_g}{1 - s_0}\right]^3$$

for the gas phase; where s_w is the water saturation, s_g is the gas saturation, and s_0 is the irreducible water saturation (Todd, 1980). In steam-water systems, the relative permeability of the vapor phase may be enhanced due to the effects of condensation and evaporation of water (Verma *et al.*, 1985).

3.3.3.2 Is this parameter site sensitive?

Due to the fractured-porous nature of the tuff at Yucca Mountain, this parameter is highly site sensitive. The complex relation between the liquid saturation and the distribution of fluid amongst the matrix and fractures results in a large uncertainty as to the appropriate form and physical significance of the relative-permeability curves.

3.3.3.3 Expected parameter variations during normal site operation

Values are uncertain. However, variations during operation will be limited to the thermally affected near-repository region.

3.3.3.4 Parameter values that may signal trouble

These are uncertain.

3.3.3.5 Role during each repository phase

During site-characterization, laboratory tests on rock cores will be conducted in order to measure the liquid-air relative permeability of the rock matrix. Concurrently, experimental work will be conducted in order to determine the effect of higher temperatures and the presence of water vapor on the relative permeability curves. Large-scale *in situ* measurements and/or block tests will be required in order to determine bulk-rock relative permeability.

Few, if any, relative permeability measurements will be made after site characterization, unless the experimental work started during site characterization is incomplete, or has identified potential problems.

3.3.3.6 Measurement conditions and potential instrumentation problems

Relative permeabilities are inferred from simultaneous measurement of the fluid flow rate(s) and hydraulic gradient(s) (Olson and Daniel, 1981; Hamilton *et al.*, 1981). Typically, one of these parameters is held at a constant value while the other is allowed to vary. Concurrently, the saturation of the liquid phase (wetting phase) is measured. Variations on the basic test procedure may include measuring temporal changes in one or more of these parameters. Measurements are repeated at numerous values of the pressure head (hence, saturation) to obtain the complete relative-permeability-characteristic curves.

In situ measurement of relative permeabilities are made using the same basic test techniques that are used in the laboratory (Olson and Daniel, 1981). However, these *in situ* tests are far less common and not as well documented as laboratory tests. Special attention must be devoted to the design and implementation of *in situ* relative-permeability tests in order to develop practical and successful measurement techniques.

Even under the best of conditions, relative permeability measurements that truly reflect the way in which a rock mass will respond to changes in saturation are difficult. Hysteretic effects, measurement uncertainties, and the lack of well-defined physical principles underlying relative permeability phenomenon, all create uncertainty when measuring and interpreting relative permeabilities. In heterogeneous formations, such as those at Yucca Mountain, the uncertainty is compounded. Additional research in this area is required before the scientific and engineering community can confidently make and correctly interpret relative permeability measurements in the fractured-porous tuff at Yucca Mountain.

3.3.3.7 What may happen if this parameter is not measured?

It is not possible to predict the rate at which radionuclide contaminated water or gases will migrate to the accessible environment without knowing the relative permeabilities. Therefore, measurements of the relative permeabilities of the liquid and gas phases are required in both the matrix and bulk-rock.

3.3.4 Water Saturation

When more than one fluid or fluid phase fills the pore space within a rock, the parameter that quantifies the degree to which a given fluid fills the pore space is called the saturation. In partially saturated groundwater systems, such as that at Yucca Mountain, the pore spaces are filled with water and gas (air and water vapor). The water saturation is given by

$$s_w = \frac{V_w}{\phi V_r} ,$$

and the gas saturation by

$$s_g = \frac{V_g}{\phi V_r} ,$$

where ϕ is the porosity of the rock (see Section 3.3.5) and V_w and V_g are the volumes of water and gas within the rock volume V_r. By the definition of saturation,

$$s_w + s_g = 1 .$$

The saturation of a rock is a macroscopic property of a lithologic unit. For instance, the water saturation within a given rock unit is the average volumetric water content, not the degree to which each pore volume is filled with water. For partially saturated rocks, the wetting fluid (water in this case) preferentially fills the small pore spaces within the rock, and the non-wetting fluid (air or steam in this case) fills the larger pore spaces. For this reason, in fractured-porous tuff, the water saturation is expected to be much higher in the matrix than in the fractures. Water filling the fractures will be concentrated at the asperities (points where the fracture walls touch).

In partially saturated rocks, the degree of water saturation is an extremely important parameter that interacts with and influences many of the other hydrologic parameters, including: relative permeability, water infiltration rate, age of water, water inflow rate, and the rate and location of groundwater recharge and discharge. Incorrect measurements and predictions of water saturation will result in erroneous conclusions regarding the rate at which radionuclides are released to the accessible environment.

There are numerous field and laboratory techniques for measuring the degree of water saturation (Morrison, 1983). The most direct laboratory techniques rely on removing the water from the sample. A comparison between the wet and dry weights yields the water saturation (Scheidegger, 1974). Other laboratory techniques rely on replacing or diluting the water in the rock sample with another fluid in order to calculate the initial water saturation (Scheidegger, 1974). Field techniques rely on measurement of indirect indicators of the water saturation, including: electromagnetic properties, rate of thermal dissipation, and nuclear response techniques (Morrison, 1983). In each case, a parameter that is sensitive to the degree of water saturation is measured. The water saturation is then calculated by comparing the measured quantity to theoretical or field-calibrated response curves. Variations in the water salinity, mineral content of the rock, and temperature effects can all create uncertainties in measured values of the fluid saturation (Morrison, 1983). Field-calibrations and repeated comparisons between field and laboratory measurements will minimize these uncertainties.

3.3.4.1 Normal parameter range

Under natural conditions, water saturation ranges from the irreducible water saturation (the water remaining in the rock when it no longer forms a continuous phase), to a value of one, for fully saturated rock. The degree of water saturation depends on the infiltration rate, recent climatic patterns, the pore size distribution of the rock (and the resultant capillary pressures), geothermal gradients, evapotranspiration rates, evaporation rates, and the proximity to the land surface or water table.

3.3.4.2 Is this parameter site sensitive?

This parameter is highly site sensitive. Water saturations ranging from 0.40 to 0.97 have been reported for rock units penetrated by two boreholes at Yucca Mountain (Sinnock, *et al.*, 1984). Irreducible saturations of 0.002 to 0.1095 have been reported for the tuffaceous units at Yucca Mountain (Peters *et al.*, 1984).

3.3.4.3 Expected parameter variations during normal site operation

In response to repository construction and operation, water saturation in the near-repository rock will probably decrease near open walls and heat sources where evaporization takes place, but may increase where recondensation takes place. However, understanding of the physical processes and fundamental mechanisms by which these changes will take place is limited by the lack of theoretical and experimental studies addressing this issue (Evans, 1983). The active research effort stimulated by the HLW program is essential for developing the conceptual and quantitative framework for predicting the thermo-hydrological response in the near-repository region. Without this we cannot accurately predict saturation changes and their influence on the ability of the repository to isolate HLW.

3.3.4.4 Parameter values that may signal trouble

These are uncertain. Significant research is needed before this question can be answered.

3.3.4.5 Role during each repository phase

During site characterization, *in situ* and laboratory tests will need to be conducted in order to measure the degree of water saturation of the rock units above, in, and below the repository horizon. It is particularly important to detect the depth to the water table and identify the tension-saturated region (region where capillary forces are strong enough to fully saturate the rock while maintaining sub-atmospheric pore pressures).

Laboratory and field measurements of saturation will continue throughout site construction in order to develop a more detailed description of the near-repository region, detect construction-induced changes, and confirm the reliability of previous measurements.

Long-term *in situ* fluid saturation monitoring, during site operation and after closure, will provide confirmation of the validity of theoretical predictions regarding the thermo-hydrological response of the rock mass. Measurements are required in the near-repository region and surrounding rock.

3.3.4.6 Measurement conditions and potential instrumentation problems

Most water saturation measurements have taken place under the auspices of soil physicists and agricultural engineers. Therefore, measurement techniques and instruments were developed for soils, rather than for hard rocks. Three factors create uncertainty in using these techniques to measure and monitor the degree of water saturation in the tuff at Yucca Mountain. The first is the fractured-porous nature of the rock, which results in a highly non-uniform distribution of saturation in the rock. The second is the influence of a large fraction of water vapor in the gas phase (resulting from elevated temperatures and perhaps, boiling). Finally, since these methods were developed primarily for sedimentary rocks, instrument response characteristics specific to the tuffaceous rocks at Yucca Mountain must be obtained.

The ability to measure water saturation and saturation changes in the tuff at Yucca Mountain will depend on developing adequate correlations between laboratory-measured saturations, saturation-sensitive physical properties of the rock, and instrument response characteristics. If sufficient care is taken to develop these relations under the anticipated range of thermal conditions, as well as the range of pore fluid chemistry and mineralogic variations, both in and around the repository, accurate measurement and monitoring of water saturation should be possible. However, developing the necessary correlations will be difficult and time consuming.

The degree to which drilling, construction, coring, and testing may alter the natural *in situ* water saturation must also be assessed. Potential influences include: 1) drilling fluid invasion into the rock matrix, 2) fracture drainage resulting from stress changes near the underground openings, and 3) evaporation or condensation of water. After assessing the degree to which these factors change the saturation of the rock, measurement techniques that avoid or compensate for these influences must be developed.

3.3.4.7 What may happen if this parameter is not measured?

This is a highly site specific parameter that is crucial to understanding the hydrologic regime at Yucca Mountain. Without measuring water saturation, the rate at which radionuclides will reach the accessible environment can not be predicted.

If changes in water saturation are not monitored throughout construction, operation, and decommissioning of the repository, it is impossible to verify theoretical predictions regarding the ability of the repository to isolate the HLW. Therefore, continual monitoring of water saturation in and around the repository rock is crucial to confirming the adequacy of the repository.

3.3.5 Porosity and Distribution of Pore Sizes

The porosity of a rock is the ratio of the void volume to the bulk rock volume. Porosity is an average property of a given rock volume and is not necessarily indicative of the size of the pore spaces within the rock. Unlike fluid flow in fully saturated rock, where it is often sufficient to know the bulk-rock porosity, description of fluid flow in partially saturated rock also requires knowledge of the pore size distribution.

In the tuff at Yucca Mountain, the porosity is created by lithophysae, fracture volume, and voids within the rock matrix, This results in highly variable porosity and a wide range of pore sizes (Scott *et al.*, 1983).

Insofar as the speed at which fluid moves from one location to another is inversely proportional to the porosity of the host rock, this parameter is critical to predicting the rate at which radionuclides will migrate to the accessible environment.

The distribution of pore sizes is the fundamental parameter influencing the partially saturated air-water relative permeability of the rock and the saturation characteristic (water retension). Although the pore-size distribution is not directly incorporated into fluid-flow models of the unsaturated zone, it is of major importance to understanding the basic physics of fluid flow and chemical transport in partially saturated groundwater systems.

There are numerous laboratory techniques for measuring the porosity of a rock, including: volumetric, optical, density, and gas expansion techniques (Scheidegger, 1974). The first three methods rely on measuring the difference between the bulk-rock and grain properties. For instance, the volumetric technique compares the volume of the bulk rock to the volume of the rock after it is crushed and compacted. Density methods, which are among the most popular, compare the bulk density to the grain density. The gas expansion method, which is the most popular technique for measuring the porosity of dry rock, directly measures the volume of gas or air in the pore space.

There are no direct methods for measuring porosity *in situ.* Instead, the porosity is estimated by interpreting geophysical well logs and/or tracer tests (Javendal, 1983). Geophysical techniques for determining porosity fall into three broad categories: density methods, nuclear methods, and resistivity methods (Javendal, 1983). Each of the techniques relies on a comparison between the bulk formation properties (rock and fluid) to the properties of either the fluid or the rock alone. Unfortunately, when the fluid saturation is also a variable, the relatively simple relations between the measured parameters and the porosity of the formation are no longer valid. Therefore, these conventional geophysical techniques are not useful methods for *in situ* porosity measurements in the partially saturated zone. Tracer tests are also a common method of determining the *in situ* porosity. The average porosity of the formation is calculated from the length of time a "tagged fluid" takes to travel from one point to another in the medium. Here again, the calculation of porosity from tracer tests is complicated by the partially saturated medium. Therefore, this method will only be useful in the saturated region underlying the repository horizon.

The pore size distribution of core-sized rock samples is usually inferred from the saturation-characteristic curve (capillary pressure *vs* saturation; see Section 3.3.6) (Scheidegger, 1974). The radii of the pores are calculated from the basic relation between the pore radius and the capillary pressure,

$$r = \frac{2\gamma\cos\theta}{p_c} ,$$

where r is the equivalent capillary tube radius that would result in the measured capillary pressure, γ is the surface tension, θ is the contact angle, and p_c is the capillary pressure. A second method for determining the pore-size distribution relies on the relation between the pore-radii and the quantity of water sorbed onto the surfaces of the rock (Scheidegger, 1974).

During a recent study, the mercury infusion method (saturation-characteristic obtained using mercury injection) was combined with the gas adsorption method to measure the pore-size distribution of several samples of granodiorite. Pore-size distributions in the range of 10^{-5} to 10^{-10} meters were reportedly measured (Evans, 1983). The success of the measurements suggests that similar procedures can be used to measure the pore-size distribution in the tuffs at Yucca Mountain. However, refinements in the laboratory technique and validation of the results (*i.e.*, comparisons among methods) is required before these measurements can be made confidently.

3.3.5.1 Normal parameter range

Porosity is a highly variable rock property. Representative values for different rock types range from 0.06 to 0.45, (Morris and Johnson, 1967). The distribution of pore sizes is also highly variable and depends on the rock type, depositional environment, and post-depositional environment.

3.3.5.2 Is this parameter site sensitive?

This is a highly site-specific parameter. Representative values of the porosity range from 0.07 to 0.11 for the welded tuff, 0.20 to 0.30 for the zeolitized non-welded tuff, and 0.40 to 0.46 for the non-welded tuff (Peters *et al.*, 1984). Average pore diameters, as determined by mercury injection tests, range from 0.013 to 0.247 μm (Peters *et al.*, 1984).

3.3.5.3 Expected parameter variations during normal site operation

Changes in porosity and pore-size distribution resulting from constructing and operating a repository at Yucca Mountain will be limited to the near-repository region. These changes, which may slightly increase or decrease the porosity, result from stress redistribution around the underground openings, fracturing of the rock at the walls of the underground openings, and hydrothermal alteration. Porosity changes in the near-repository rock are not expected to lessen the ability of the repository to isolate the HLW (Sinnock *et al.*, 1984).

3.3.5.4 Parameter values that may signal trouble

These are uncertain.

3.3.5.5 Role during each repository phase

The porosity and pore-size distribution is one of the most important parameters for assessing the transport characteristics of partially saturated rock. Both laboratory and field measurements are required to determine these parameters. Laboratory measurements on cores from boreholes and excavations will be made in order to determine the porosity and pore-size distribution of all the important hydrostratigraphic units in the partially saturated zone. Field measurements (tracer tests and geophysical techniques) will be used to determine the porosity of the fully saturated hydrostratigraphic units underlying and surrounding the repository.

After site characterization, the porosity and pore-size distribution may continue to be measured on cores from newly excavated rock, but the measurements will be used mainly to confirm the validity of previously determined values. Changes in this parameter, due to construction and operation, are expected to be small. Therefore, ongoing monitoring of this parameter is not required.

3.3.5.6 Measurement conditions and potential instrumentation problems

Laboratory and *in situ* techniques for determining porosity and pore-size distribution were developed primarily for evaluating soils and sedimentary rocks. Applying these same techniques to a highly-heterogeneous igneous rock is hindered by conceptual uncertainties and practical difficulties. The uncertainties result primarily from the lack of experimental confirmation that the same conceptual framework is appropriate for characterizing igneous rock that is suitable for a relatively unconsolidated soil. Practical difficulties result from the lack of well established laboratory procedures for making these measurements in hard (*i.e.*, low-permeability) rocks, and from the lack of guidelines for identifying the appropriate "representative" volume of rock to test (Peters *et al.*, 1984). In order to improve our confidence in these measurements and understand the role of these parameters in controlling fluid flow in tuffaceous rocks, site-specific correlations between laboratory and field measurements, as well as experimental validation of these techniques and concepts are required.

3.3.5.7 What may happen if this parameter is not measured?

This parameter is highly site-specific. If it is not measured, it is impossible to predict the rate at which radionuclides will migrate to the accessible environment.

3.3.6 Saturation Characteristic Curve

The saturation characteristic curve (sometimes called the moisture retention curve) relates the degree of water saturation to the capillary pressure in the water-filled pore spaces of the rock (sometimes called the moisture suction or matric potential). With increasing capillary pressures, the larger pore spaces drain, thereby reducing the degree of saturation. In general, the degree of saturation is not a single-valued function of the capillary pressure; hysteretic effects (*i.e.*, depending on whether the measurement is made during drying or imbibition) create significant differences in the relation between these two parameters.

The highly heterogeneous nature of the tuff units at Yucca Mountain results in a wide range of saturation-characteristic curves (Peters *et al.*, 1984). The variation results from the different pore structure of the welded, non-welded, and zeolitized tuffs. However, the properties are variable even within a given unit. In general, the non-welded units have low moisture retention characteristics and the welded units, high retention characteristics.

The saturation characteristic is one of two fundamental properties that is required input for fluid flow-models of partially saturated rocks. Therefore, it is of primary importance to predicting the consequences of locating a HLW repository in a partially saturated hydrologic regime. Insofar as the saturation characteristic quantifies the ability of a medium to retain water in the pore spaces, it interacts with several of the other critical hydrologic parameters, including: fluid velocities, water infiltration rate, age of water, and water inflow rate.

The saturation characteristic curve is measured in the laboratory on core-sized (or smaller) rock samples obtained from boreholes and excavations. The most common technique for making this measurement is the mercury infusion method. The characteristic curve is obtained by injecting mercury (a non-wetting fluid) into the core at progressively higher pressures while simultaneously measuring the volume of mercury (hence, the saturation) that has invaded the core. The water-saturation characteristic curve is then related to the mercury-injection curves by the relations:

$$s_w = 1 - s_{Hg} \quad ,$$

and

$$p_c = p_{Hg} \frac{\gamma_w \cos(\theta_w)}{\gamma_{Hg} \cos(\theta_{Hg})} \quad ,$$

where s_w and s_{Hg} are the saturation of water and mercury, p_c is the capillary pressure, p_{Hg} is the pressure at which the mercury is injected, γ_w and γ_{Hg} are the surface tensions, and θ_w and θ_{Hg} are the contact angles.

Recently, a more direct method has been used to measure the saturation characteristic curves of the tuffaceous rocks at Yucca Mountain (Peters *et al.*, 1984). Total potential was measured directly with a thermocouple psychrometer (see Section 3.3.7, Water Potential) while the water saturation was determined gravimetrically. Saturation of the sample was changed by progressively drying the rock in a microwave oven. One of the drawbacks of this technique is that the thermocouple psychrometers measure the total potential, which is the sum of the matric (capillary pressure) and osmotic (solute) potential. Therefore, the pore-fluid chemistry and changes in the pore-fluid chemistry may influence the results of the test, resulting in erroneous interpretation of the data.

Another technique for measuring the saturation characteristic curves requires using a centrifuge to expel water from a core sample (Ward and Morrow, 1985). The corresponding capillary pressure is calculated from the rotational speed of the centrifuge and the length of the rotor arm. Although this method is still in an experimental stage, validation against other techniques shows that it holds promise as a valuable technique for routinely measuring saturation characteristic curves in very-low permeability hard-rocks (Ward and Morrow, 1985).

3.3.6.1 Normal parameter range

This is an extremely site- and medium-specific property. Until a significant number of measurements are made on tuffaceous rocks, it is not possible to specify the "normal range."

3.3.6.2 Is this parameter site sensitive?

This parameter is highly site-sensitive. Measurements on 48 samples of the tuffaceous rocks at Yucca Mountain have been reported by Peters *et al.* (1984). Representative saturation characteristic curves have been chosen for the densely welded tuff, vitric non-welded tuff, and the zeolitized non-welded tuff; non-welded units desaturate quickly at capillary pressures in the 4 to 10 bar range, welded units drain gradually over a range of several to over 1000 bars, and the zeolitized non-welded units desaturate gradually over a range of several to over 10,000 bars (Peters *et al.*, 1984). However, the wide range of saturation characteristic curves within each of these rock types indicates that additional measurements are required in order to develop truly representative curves.

3.3.6.3 Expected parameter variations during normal site operation

Since the saturation characteristic curve depends on the pore-size distribution and the physical properties of the fluid in the pore-space, any thermally sensitive property of these two factors may be expected to change the saturation characteristic when the temperature in the near-repository rock changes (Constanz, 1983). The influence of temperature on the moisture retention characteristics is well known; as the rock gets hotter, the moisture retention capability decreases. However, the simple capillary retention theories currently available for quantifying this phenomena are inadequate (Constanz, 1983). Both an experimental evaluation of the phenomena and a theoretical explanation for the mechanism must be obtained before the expected variation in this parameter can be quantified.

3.3.6.4 Parameter values that may signal trouble

These values are uncertain.

3.3.6.5 Role during each repository phase

During site characterization, laboratory tests will be conducted to develop saturation characteristic curves for all of the hydrostratigraphic units in the partially saturated region in and around the repository. Concurrently, experiments will be performed to determine the sensitivity of the curves to the temperature and the state-of-stress.

Few, if any, saturation characteristic curves will be measured after the site characterization phase is complete.

3.3.6.6 Measurement conditions and potential instrumentation problems

Until recently, saturation characteristic curves were measured primarily in soils and sedimentary rocks. Therefore, the experimental set-up for testing tuff samples may require modification of the conventional set-up to allow for testing throughout the appropriate capillary pressure range. Recent tests on 48 tuff samples indicate that such an apparatus is available, and that saturation characteristics can be measured (Peters *et al.*, 1984). Nevertheless, comparisons between the mercury infusion technique data and data from the more direct psychrometer methods show that the agreement between the two methods is not very good. The centrifuge technique may provide an alternative that would allow validation of these measurements and resolution of the discrepancies between them.

A second difficulty associated with measuring a saturation characteristic curve for tuff results from the lack of guidelines for identifying the representative sample size. Very small samples are typically used (less than several cm^3). The large variation in saturation characteristics measured using such small samples (Peters *et al.*, 1984) suggests that larger samples are needed in order to obtain representative values for these curves. Additional testing will help to resolve this issue, provide guidelines for choosing the appropriate volume of the rock to test, and develop procedures for testing larger rock samples.

3.3.6.7 What may happen if this parameter is not measured?

It is impossible to predict the rate at which soluble radionuclides will migrate to the accessible environment if this parameter is not measured.

3.3.7 Water Potential

The total fluid potential (ϕ_t) is defined as the sum of the potential due to three components.

$$\phi_t = \phi_p + \phi_g + \phi_o \ ,$$

where ϕ_p is the matric potential or pressure head, ϕ_g is the gravitational potential, and ϕ_o is the osmotic potential. The gravitational potential per unit volume is given by

$$\phi_g = g \int_0^z \rho dz \ ,$$

where ρ is the density of the fluid, g is the acceleration due to gravity, and z the elevation above a given datum. In the saturated zone, the pressure potential (fluid pressure) is the result of the pressure exerted by the column of water above the measuring point, and is given by

$$\phi_p = g \int_0^h \rho dh \ ,$$

where h is the hydraulic head. In the partially saturated zone, ϕ_p (commonly referred to as the matric potential) is negative, and results from capillary and adsorptive forces that tend to bind the water to the host rock. The osmotic potential, ϕ_o, is the result of the presence of solutes in the pore water.

Insofar as potential gradients result in the flow of water and solutes, and the hydraulic properties of the rock are a function of potential, the potential interacts with all of the the critical hydrologic parameters. Accurate potential measurements, both in the laboratory and in the field, are essential to understanding the natural flow regime at Yucca Mountain as well as predicting and monitoring the response of the hydrologic system to thermal loading.

In the saturated region, the pressure potential (at a given location) is measured by lowering a pressure transducer into a borehole and allowing it to equilibrate with the pore pressure of the surrounding rock. If a single borehole is used to measure the potential at several depths, packers are required in order to isolate the interval in which a measurement is being made. In this case, care must be taken to ensure that the packer seals are tight, and that the pressure in the isolated zone between the packers is fully equilibrated with the formation before the measurement is made.

In the partially saturated zone, measuring the pressure potential is not so straight forward. The measurement technique depends on the value of the parameter. For small negative potentials (less than 1.0 bar), a tensiometer is commonly used to measure matric potential in soils (Hillel, 1980a). The tensiometer measures the matric potential by allowing the pressure in a closed container to equilibrate with matric potential of the soil. A porous cup, which allows transfer of pore-water and solutes in and out of the vessel, prevents air from entering the container. Since solutes are free to move in and out of the vessel, the concentrations in the soil and vessel eventually equilibrate. Therefore, tensiometers generally measure only the matric potential. The pressure in the vessel can be measured with a manometer or any one of a number of pressure transducers. Tensiometers have been used extensively for many years by soil scientists and geotechnical engineers. If carefully installed, to ensure good contact between the ceramic cup and the soil, reliable matric potential measurements, in the range of 0.0 to −0.8 bars, can be obtained (Hillel, 1980a and Morrison, 1983).

A second version of the tensiometer, the osmotic tensiometer, has been used with mixed success to measure matric potentials ranging from 0 to −15 bars (Peck and Rabbidge, 1969) and more recently from 0 to −2 bars (Evans, 1983). Recent developments of this technique are discussed by Evans (1983).

For high matric potentials (−0.9 to −72 bars), thermocouple psychrometers (Morrison, 1983 and Hillel, 1980a) and heat dissipation probes (Montazer, personal communication) are used to measure potential. Thermocouple psychrometers measure the relative humidity of the pore spaces in the rock, which can be related to the potential (matric plus osmotic) by

$$\phi_p + \phi_o = \frac{RT}{V} \ln \frac{p}{p_o} ,$$

where p/p_o is the relative humidity, R is the ideal gas constant, T is the absolute temperature, and V is the molar volume of water (Morrison, 1983). In some cases, a salinity detector, for determining the osmotic potential, is used in conjunction with a thermocouple psychrometer. The osmotic potential can be calculated to within 10% and subtracted from the value measured with the thermocouple psychrometer in order to calculate the matric potential (Morrison, 1983). Detailed descriptions of several thermocouple psychrometers are given by Morrison (1983) and Evans (1983). Recent field applications of this technique for measuring the potential in fractured rock are discussed by Evans (1983).

3.3.7.1 Normal parameter range

This is a highly site sensitive parameter. Measured values range from a fraction of a bar to many tens of bars. Typical values for hard rock in the unsaturated region are largely unknown due to a lack of measurements in this environment.

3.3.7.2 Is this parameter site sensitive?

This parameter is highly site sensitive. Matric and/or matric plus osmotic potentials from the USW UZ-1 borehole at Yucca Mountain range from −0.4 bar to nearly −30 bars (Montazer *et al.*, 1985).

3.3.7.3 Expected parameter variations during normal site operation

This is uncertain.

3.3.7.4 Parameter values that may signal trouble

This is uncertain.

3.3.7.5 Role during each repository phase

The matric and total potentials will be measured in the partially saturated region above, below, and in the repository horizon during the site characterization phase. The potential will also be measured in the laboratory to establish the saturation and relative permeability characteristic curves of the tuffaceous rock units. Routine monitoring of the potential in the repository horizon and surrounding rock units will continue throughout the construction and operation phases to confirm the reliability of earlier measurements, detect any repository-induced

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changes, monitor groundwater movement in the partially saturated zone, and validate performance predictions.

In the saturated zone, the pressure potential (or head) will be measured throughout the groundwater basin during the site characterization phase in order to infer flow directions and calculate flow velocities. During site characterization, fluid pressure will also be measured in conjunction with the flow tests that are used for calculating the hydraulic properties of the saturated tuffs. Routine monitoring, at selected locations, will continue throughout the construction, operation, and post-closure phases in order to detect repository-induced changes, monitor groundwater movement in the saturated region, and validate performance predictions.

3.3.7.6 Measurement conditions and potential instrumentation problems

Conventional instruments for making potential measurements are satisfactory for the saturated zone. However, the long-term stability and reliability of pressure transducers, as well as the reliability of borehole seals and packers, need to be investigated. In addition, if temperature changes are anticipated in the saturated region, the influence of these changes on the operation and calibration of the pressure transducers should be investigated.

Conventional instruments for making *in situ* potential measurements in the unsaturated zone are intended for use in soils, rather than hard rock. Therefore, conventional techniques may not be directly applicable to the repository environment. For instance, techniques that require contact between the sensing element and the rock or soil (such as use of tensiometers) are not well suited in hard rock.

In boreholes, potential measurements are obtained by isolating a section of the borehole (with packers, for instance) and allowing the borehole to thermodynamically equilibrate with the surrounding rock. Once in equilibrium, thermocouple psychrometers can be used to measure the total potential. Since the borehole is relatively large compared to the pore spaces, it may take several months before the borehole equilibrates with the surrounding rocks (Evans, 1983). Experience indicates that there are many practical problems associated with the use of thermocouple psychrometers (Morrison, 1983; Evans, 1983). It is anticipated that these will be exacerbated by the long-term monitoring required to confirm repository performance predictions. Difficulties are caused by the limited range of the sensor, thermal gradients between the reference and sensing thermocouples, contamination (deposition) of the thermocouple, and corrosion of the thermocouple (Morrison, 1983).

Ongoing research programs aimed at measuring fluid potential and potential-related parameters will improve the accuracy and reliability of making these measurements.

3.3.7.7 What may happen if this parameter is not measured?

Without measuring the potential it is not possible to determine groundwater flow directions, establish the fundamental hydrologic properties of the rock units, or monitor flow directions during and after the repository operations phase. Therefore, it is essential to measure this parameter.

3.3.8 Water Infiltration Rate

The water infiltration rate is defined as the quantity of water (volume/unit area/unit time) that seeps through the ground surface and travels horizontally or vertically towards the water table. The water infiltration rate is estimated using one or more of several methods. Information on the climatic, topographic, and vegetation conditions at the site can be combined to estimate the surface runoff, annual rainfall, and the evapotranspiration rate. By taking the difference between the annual rainfall, and the sum of the runoff and evapotranspiration, the infiltration rate can be estimated. A second method uses a mass balance for the groundwater basin to estimate the amount of infiltration that must occur for the water table to exist in its present state. Both methods provide an approximate value for the water infiltration rate, as they do not consider local variability in rainfall, runoff, and soil properties.

More precise estimates of the water infiltration rate are obtainable by analyzing the potential, saturation, and hydraulic properties of the rock units. The simplest calculations made by this approach, assume a one-dimensional steady-state infiltration. Under these conditions, the infiltration rate equals the effective hydraulic conductivity, $kk_{rw}\rho g/\mu$, where k is the intrinsic permeability, k_{rw} is the relative permeability to water at a given saturation, ρ is the fluid density, g is the acceleration due to gravity, and μ is the fluid viscosity (Hillel, 1980). More complex applications of this type of technique include the effects of one or more of the following: thermal gradients, transient flow, multidimensional flow, water vapor transport, and the variability of the hydraulic, lithologic, and geologic properties of the rock units (Hillel, 1980; Rulon and Bodvarsson, 1985; Sass and Lachenbruch, 1982; Ross, 1984). Analytic or numerical methods are used to duplicate the observed conditions. When a satisfactory match is obtained between observed data (*e.g.*, potential, and saturation) and theoretical predictions, it is assumed that the correct infiltration rate has been used for the calculations.

3.3.8.1 Normal parameter range

Infiltration rates are highly variable, and depend on a number of factors, including: rainfall, humidity, vegetation, topography, and the physical properties of the surface soils.

3.3.8.2 Is this parameter site sensitive?

This parameter is extremely site sensitive. Estimated groundwater recharge rates at Yucca Mountain range from 0.5 to 10 mm/yr (Sass and Lachenbruch, 1982; Rice, 1984; Rulon and Bodvarsson, 1985; Montazer and Wilson, 1984; Sinnock *et al.*, 1984). However, hydraulic conductivity data, combined with steady-state infiltration calculations, suggest that the infiltration rate may be considerably lower than 0.5 mm/year (Peters *et al.*, 1984; Rulon and Bodvarsson, 1985).

3.3.8.3 Expected parameter variations during normal site operation

This parameter will be influenced primarily by climatic changes, rather than the operation of the repository. Paleo-climatic studies that address this issue are currently underway (Spaulding *et al.*, 1984).

3.3.8.4 Parameter values that may signal trouble

Infiltration rates that result in resaturating the host rock, or the lithologic units above or below it, are undesirable. Additional research and site investigations are required before a meaningful resolution of this issue is available.

3.3.8.5 Role during each repository phase

The water infiltration rate should be evaluated during every repository life phase. Estimates of the infiltration rate are initially required for the site characterization and feasibility analyses. Thereafter, the infiltration rate should be one of a set of routinely monitored parameters. In the unlikely event of temporary resaturation of the host rock or overlying horizons, routine monitoring of the infiltration rate will allow engineered safety measures to be taken in a timely manner.

3.3.8.6 Measurement conditions and potential instrumentation problems

Four major difficulties create uncertainty when the above-mentioned techniques are used to calculate the water infiltration rate. First, all results strongly depend on the relative permeability and saturation characteristic curves of the rock. As mentioned in Sections 3.3.3 and 3.3.6, there is considerable uncertainty associated with measuring and assigning values to these parameters. Second, the role of major through-going fractures and the spatial variability of properties of the surficial material are uncertain. Third, during infiltration, the interaction between and the role of the porous matrix and the fractures, in a fractured-porous medium, is poorly understood. Finally, the low infiltration rates at Yucca Mountain make applying any of these techniques more difficult.

3.3.8.7 What may happen if this parameter is not measured?

Since the infiltration rate is the parameter governing the rate and location at which radionuclides enter the groundwater system, and thereby travel to the accessible environment, it is unthinkable that it not be measured.

3.3.9 Water Inflow Rate

The water inflow rate is defined as the rate at which water enters the excavated openings and boreholes. In the partially saturated rocks at Yucca Mountain, the water inflow rate will have three components. The first of these results from locally perched water that may be intersected by the shafts, boreholes, and excavations. Inflow usually occurs where a fault intersects a borehole or excavation (Fernandez and Freshley, 1984). This water will flow into the openings if sufficient vertical or horizontal pressure gradients develop. With time (typically several months), the inflow rate will decrease, until the water supply is depleted (Fernandez and Freshley, 1984). The second source of water inflow will result from water vapor transport from the rock surfaces to the underground openings. The third and last source of water inflow results from thermally and stress induced changes in the water saturation. If the rock becomes saturated locally and this region is accessible to repository openings, water inflow may result. Experimental data show that significant inflow of water into the underground openings may occur during thermal loading (Nelson *et al.*, 1981; Zimmerman, 1982; Rogue and Binnall, 1983).

3.3.9.1 Normal Parameter Range

The normal range of this parameter is uncertain, as is the degree to which each of the components contributes to the total water inflow rate.

3.3.9.2 Is this parameter site sensitive?

This parameter is extremely site sensitive. In fact, the parameter is sensitive to geologic and hydrologic variations within the tuffaceous units.

3.3.9.3 Expected parameter variation during normal site operation

This is uncertain. However, the water inflow rate is expected to increase during the initial thermal loading of the respository (Pruess *et al.*, 1984). As the near-repository rock dries, the water inflow rate may decrease, depending on a number of factors (Pruess *et al.*, 1984). After the primary thermal pulse decays, the water inflow rate may again increase due to spatial variations in the resaturation of the near-repository rock.

3.3.9.4 Parameter values that may signal trouble

These values are uncertain. The interaction between this parameter and a number of other parameters, including canister corrosion, temperature of the repository, convective heat transfer, and fluid velocity is complex. Additional research in this area will provide the much needed answers to the questions regarding the interrelation of these parameters.

3.3.9.5 Role during each repository phase

Water inflow into the repository will be monitored throughout the site characterization, site construction, and operational phases.

3.3.9.6 Measurement conditions and potential instrumentation problems

The techniques used to measure the water inflow are rate dependent. If the rate is large enough to require that it be pumped from the repository, conventional flowmeters, of which there are a wide variety, can be used. For low inflow rates, the water is collected in containers and the humidity of the air leaving the ventilation system is measured (Witherspoon *et al.*, 1980). In general, low inflow rates are difficult to measure on a continuous basis with the techniques and instruments used today. Water inflow typically occurs over a large surface area, rendering collection and rate measurement difficult.

3.3.9.7 What may happen if this parameter is not measured?

Water inflow rate is an important parameter that has a significant impact on a number of other parameters, most notably on the canister corrosion rate and the temperature of the near repository rock. Vital information, influencing the entire operation of the repository, will not be available if this parameter is not measured.

3.3.10 Fluid Velocity

The fluid velocity is defined as the true particle (water or solute) velocity in the fractures and pore spaces of the rock. In a fully saturated system, the average linear velocity is equal to the flux divided by the effective porosity (interconnected pore spaces). In a partially saturated system,

$$v_{ave} = flux / \phi_{effective} \quad ,$$

where $\phi_{effective}$ is the fractional volume of water-filled pore space.

In some cases, fluid and/or solute velocities are measured directly by observing the time it takes for a "tagged" packet of water to move from one location to another. However, fluid velocities (average linear velocity) are usually calculated indirectly, based on potential gradients, effective permeabilities, and the effective porosity of the rock. The distribution of fluid velocities around the average is commonly accounted for by the hydrodynamic dispersion coefficient. This coefficient can be measured in the laboratory and in the field. Field-measured values are usually much larger than laboratory measured values, due to the heterogeneity of subsurface rocks or sediments (Freeze and Cherry, 1979; Guven *et al.*, 1985). Considerable controversy exists over the physical significance and validity of the hydrodynamic dispersion coefficient in modeling groundwater systems.

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3.3.10.1 Normal parameter range

Fluid velocities are highly variable and site-specific. Therefore, typical values are not applicable to site-specific applications.

3.3.10.2 Is this parameter site sensitive?

This parameter is site and hydrostratigraphic unit specific. Values for the saturated region range from 1 to 50 m/yr (Sinnock *et al.*, 1984). Fluid velocities in the partially saturated region are not established at this time.

3.3.10.3 Expected parameter variations during normal site operation

These variations are uncertain.

3.3.10.4 Parameter values that may signal trouble

Since the solute-laden water will traverse numerous hydrostratigraphic units while traveling to the accessible environment, maximum velocities must be specified for each of these units. This information is not available at this time.

3.3.10.5 Role during each repository phase

During site characterization, *in situ* measurements of the fluid velocity will be attempted in the saturated region. In addition, measuring fluid velocities (infiltration) in the partially saturated zone by direct and indirect techniques will also be attempted. As part of these investigations, effective porosities, effective permeability, saturation, and water potential measurements will also be made (see Sections 3.3.2, 3.3.3, 3.3.4, 3.3.5, and 3.3.7). During the operation phase, measurements will continue for the purpose of verifying previously measured values and detecting operation-induced changes of this parameter. Long-term monitoring of the parameters required for estimating fluid velocities (*i.e.*, potential, temperature, and saturation) should continue indefinitely.

3.3.10.6 Measurement conditions and potential instrumentation problems

In the saturated zone, direct measurement of the average *in situ* fluid velocity is usually done by observing the travel time of chemical tracers in the rock mass. Two techniques are commonly used: natural gradient tests and imposed gradient tests.

Natural gradient tests can be conducted using one or more boreholes. In the single borehole method (commonly called the point dilution method), a known concentration of a trace chemical is put into the borehole. The rate at which the concentration decreases with time can be related to the average linear velocity of the fluid in the formation (Drost *et al.*, 1968). In the multiple-borehole method, the tracer is injected into one borehole and fluid is sampled from one or more additional boreholes (Todd, 1980). In this manner, the average linear tracer velocity can be directly measured.

Imposed gradient tests are used to infer the transport properties (dispersivity and stratification) of the rock under a known hydraulic gradient. Single-well tests are conducted by injecting and then withdrawing the tracer. This technique is used to measure the dispersivity of rock units (Guven, 1985). Multiple borehole tracer tests are usually conducted by injecting a slug of tracer into one borehole while pumping and sampling fluid from a second borehole. Additional monitoring wells, midway between the two primary wells may also be used. In this manner, the stratification and dispersivity of the rocks can be determined. Although many different chemicals have been used as tracers, the search for an ideal general-purpose tracer continues (Apps *et al.*, 1979; Thompson *et al.*, 1974; Grisak *et al.*, 1977; Freeze and Cherry, 1979).

Indirect methods for determining fluid velocities require measurements of permeability, relative permeability, saturation, porosity and pore-size distribution, and water potential. Refer to Sections 3.3.2, 3.3.3, 3.3.4, 3.3.5, and 3.3.7, respectively, for detailed discussions regarding the measurement conditions and potential instrumentation problems of the individual parameters.

3.3.10.7 What may happen if this parameter is not measured?

This is the single-most important parameter governing the rate at which radionuclides are released to the accessible environment. Therefore, initial characterization of the flow field, followed by long-term monitoring, is essential.

3.3.11 Groundwater Recharge and Discharge

For a repository in the partially-saturated zone, the total quantity of water that will come in contact with the repository, and carry soluble

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radionuclides to the accessible environment, is governed by the rate at which meteoric water infiltrates through the overlying rock (see Section 3.3.8). The rate at which dissolved radionuclides travel to the accessible environment is governed by the flow-path to the saturated zone and, thereafter, by the regional groundwater flow. Once in the saturated zone, the solute-laden water will travel down-gradient towards local sinks (*e.g.*, pumping wells) or to regional groundwater sinks. Therefore, the rate and location at which radionuclides enter the accessible environment is governed to a large extent by the location and rate of aquifer recharge and discharge. Groundwater sources (recharge) and sinks (discharge) are identified from the location of surface outcrops of the individual rock units, pressure head distributions (see Section 3.3.7), groundwater use, and the distribution of chemical species in the groundwater (see Section 3.4.1). Recharge and discharge rates are estimated from the mass balance for the groundwater basin, permeability and potential gradients (see Sections 3.3.1, 3.3.2, and 3.3.7), and groundwater use measurements. Aside from meteoric water infiltration measurements (which are discussed in Section 3.3.8), assessing the rate and location of aquifer recharge and discharge at Yucca Mountain requires only straightforward application of conventional hydrological techniques.

3.3.12 Seal and Backfill Properties

The hydrologic properties of the repository seals and the backfill material surrounding the waste canisters will be one of the critical factors in controlling radionuclide containment if the canister is breached and waste form leached by the groundwater. If not sufficiently impermeable, repository seals may provide short-cuts whereby infiltrating waters can rapidly reach the canisters and then travel on to the accessible environment (Fernandez and Freshley, 1984). Backfill materials, if used, will be designed to provide a capillary barrier and adequate drainage of water away from the canister (Fernandez and Freshley, 1984). *In situ* and laboratory tests will be conducted to determine the effect of heating, drying, resaturation, and chemical interactions on the hydrological properties of the materials. (Refer to Sections 3.3.2, 3.3.3, and 3.3.4 for discussion of required measurements.)

3.4 Geochemical Parameters

There are several issues to be addressed when considering the isolation of high-level waste (HLW) in tuff which are resolvable by chemical studies:

1. Groundwater components, which influence the volatility, solubility, and colloid forming properties of radionuclides, and hence their transport.
2. The age of water, which indicates the rate of groundwater flow.
3. The sorptive capacity of the formation rock, which determines the degree which radionuclide transport may be retarded in this section of its leakage path.
4. The solubility and volatility of radionuclide chemical species that might form spontaneously or by interaction with groundwater or atmospheric chemicals.
5. Oxygen and water fugacity of the gases in any backfill or cavity in the repository, which influence canister corrosion and radionuclide solubility.
6. The sorptive capacities of the backfill and seals, which determine the degree which radionuclide transport may be retarded in this section of the leakage path.

In large measure, addressing these concerns requires fundamental scientific knowledge (*e.g.*, the solubility of actinide oxides) or the results of applied research (*e.g.*, the rate of corrosion under given conditions). These are scientific issues, and not directly issues of instrumentation. Such scientific issues will be discussed here only insofar as necessary to define critical parameters and their corresponding measurement and instrumentation needs. Solubilities and corrosion rates are themselves functions of temperature, oxidation potential (Eh), pH, and groundwater composition. These are parameters that must be measured meaningfully to apply the results of basic and applied research to predicting repository performance, which is where instrumentation comes in. Changes in groundwater chemistry caused by radiolysis are considered under the topic of Canister and Support System Corrosion (Section 3.4.6).

Some chemical parameters are determined by laboratory procedures that require only routine instruments, but because of procedural intricacies require correct methods and proper execution to yield good results. We include discussion of some of these techniques in this review.

It is certain that during site characterization, repository construction, and operation and retrievability, *in situ* studies of such things as the repository environment, and canister corrosion, will be conducted. In preparing this review, we have attempted to anticipate what these studies might involve, and what the associated instrumentation needs might be.

Report NUREG/CR-3062, "Status of Geochemical Problems Relating to the Burial of High-Level Radioactive Waste, 1982" (Apps *et al.*, 1983) was used as a source of information about the general geochemical issues related to nuclear waste isolation.

3.4.1 Groundwater Chemistry

The groundwater chemistry breaks down into a number of subparameters. Eh, or oxidation-reduction potential, and pH are of primary importance in determining the solubility of many transition metal radionuclides. The higher oxidation states of metals are more soluble. The hydroxides of most metals are relatively insoluble, so that at lower pH (lower hydroxide ion concentration) the hydroxides will be more soluble than at higher pH.

Eh has the dimension of volts and can be either measured directly or calculated indirectly. Direct measurements are unreliable because of electrode overvoltages or nonequilibrium conditions in the system being measured. This last condition is particularly important in a system as vast as a repository. Eh is usually calculated by putting concentration values of redox couples, usually ferrous-ferric or sulfur-sulfate, into the Nernst equation, such as,

$$E = \frac{RT}{F} \ln \frac{[\mathrm{Fe}^{+2}]}{[\mathrm{Fe}^{+3}]} \ ,$$

where E is the potential in volts, R is the gas constant, T is the absolute temperature, and F is the Faraday constant.

However, because the voltage depends on the ratio of concentrations, by itself Eh tells nothing about the quantity of radionuclides the rock formation can be expected to reduce. To do this, the rock must be analyzed for the concentration of each member of the redox couple of interest. There are several redox couples commonly used to determine Eh. These are Fe^{+2}-Fe^{+3}, S^0-S^{+4}, S^{-2}-S^0, and Mn^{+2}-Mn^{+4}.

Although it might seem that exposure to atmospheric oxygen during sampling would perturb the ratios of redox couples in rocks, this can be avoided by making powdered samples from bulk ones in anoxic conditions. Based on crystal geometries of minerals in the repository formation, a calculation of the surface concentration of the reducing species can be made. This datum can then be used to estimate the reductive capacity of fracture surfaces in the far-field where oxygen will not have penetrated.

Important secondary parameters are the concentrations of ions which complex with the transition metals among the waste radionuclides. Carbonate, sulfate, chloride, and fluoride ions complex with metal ions, increasing metal solubility. Certain organic compounds that could be introduced into a repository by human activity also complex with metal ions, with the same effect.

The effect of trace components of groundwater, those with concentrations on the order of less than one part per million, is not important. An exception is aluminum, which, because it is a trivalent ion with a high-charge density, is a powerful inducer of colloid flocculation. Mole for mole, it is expected to have a flocculating effect 100 times stronger than that of divalent ions such as calcium, and 10,000 times stronger than monovalent ions such as sodium. One ppm of aluminum will have the same flocculating power as 8500 ppm of sodium. The concentration of aluminum in groundwater can influence the migration of radiocolloids which might form.

In the future, it will be important to monitor radionuclides and their decay products which leak from the repository into groundwater. Since some of these elements are occasionally found in groundwater, analyses for background concentration must be made (see Section 3.2.2, Naturally Occurring Radionuclides). The important naturally occurring radionuclides are uranium, thorium, and radium. Naturally stable elements with radioactive isotopes occurring in HLW, include: cesium, iodine, lead, selenium, tin, and palladium.

Groundwater chemistry must be determined during the site characterization phase, and monitored during site construction and operations phases to determine if human activity has induced any changes. This includes the effects of radiolysis on groundwater chemistry.

When examining tuff formations, there are two types of groundwater that must be investigated. First, there is infiltrating water, which starts at the surface and percolates into the unsaturated zone of the formation. It may be sampled in the exploratory shaft driven during the site characterization. Second is the water of the saturated zone. It may be collected for analysis after boring sampling wells. This field activity should be coordinated with hydrologic field studies.

3.4.1.1 Interaction with other parameters

The nongeochemical parameter that has the greatest effect on groundwater chemistry is temperature. The solubility of most solid materials increases with higher temperature. Over the post-closure history of a repository, changes in temperature will have significant effects on groundwater chemistry. Scenarios are conceivable in which these chemical changes would affect the hydrologic properties of the formation. Hot water flowing through rock pores or fractures may dissolve enough material to increase their dimensions and significantly increase water flow rate through the rock As the water cools, material may be precipitated in pores or fractures in amounts sufficient to decrease flow rates. These two scenarios could occur sequentially in different sections of the rock formation. Dissolution of rock may also alter its mechanical properties.

Study of groundwater chemistry should be coordinated with hydrology studies. The chemical composition of groundwater often provides important clues to the history of this water, its flow path, and time of travel.

Calcium combines with fluoride, carbonate, or sulfate to form insoluble compounds. A high concentration of calcium necessarily means a low concentration of the others. In the case of calcium carbonate, magnesium and pH are also important factors.

A consideration to keep in mind is that the groundwater chemistry will be altered as groundwater dissolves materials from the repository. Groundwater migrating back out of the repository will be different from what it was when it entered. The major changes will result from ion exchange with backfill materials, which cannot be defined at this time. After the backfill material is completely loaded, leaking dissolved radionuclides will be available to alter the groundwater chemistry. Some of the available radionuclides will complex with groundwater anions.

3.4.1.2 Normal parameter range

The pH for groundwaters range from 3.0 to 9.5. The range of Eh is from −0.4 volts (reducing) to +0.7 volts (oxidizing) (Bass Becking *et al.*, 1960). The range of concentration of chloride in groundwater is usually a few tens of parts per million, but it can be as high as a few tens of thousands of ppm in some brines. The range of sulfate or magnesium is usually up to several tens of ppm but can be a few hundred ppm in limestone areas. The concentration of calcium is usually several tens of ppm. The concentration of fluoride is usually less than one ppm, but it can be as high as a few tens of ppm (White *et al.*, 1963). The range of anthropogenic organic chemicals cannot be assessed *a priori.*

3.4.1.3 Is this parameter site sensitive?

The concentration of dissolved materials in groundwater depends very much on the composition of the rock through which it traveled. This parameter is site sensitive.

3.4.1.4 Expected parameter variations during normal site operation

Except for Eh and anthropogenic organics, these subparameters should not vary during normal site operation. Eh will necessarily increase as the repository rock is exposed to oxygen from air in the tunnels. The concentration of anthropogenic organics may vary depending on the nature and extent of spills of such materials and the thoroughness of cleanup operations. Variations due to increased temperatures have been discussed in Section 3.4.1.1, Interaction with other parameters.

3.4.1.5 Parameter values that may signal trouble

Interactions among these subparameters are complex, but several computer codes exist that can predict the solubilities of various metals, given the groundwater composition.

3.4.1.6 What may happen if this parameter is not measured?

Without knowledge of the groundwater chemistry, the solubilities of radionuclides cannot be accurately predicted.

3.4.2 Age of Water

The age of water is an indicator of its travel time through the rock upstream from the sampling site. If the upstream and downstream formations are of similar permeability and mineralogy a prediction of the travel time of a plume of radioactive waste leaking from a repository can be made.

The instrumental parameter used in determining the age of water is the concentration of various isotopes. Concentrations of radioisotopes such as tritium, ^{14}C, or ^{36}Cl are measured using appropriate radiation counters or, for more sensitive measurements, a tandem accelerator–mass spectrometer. These are compared with their concentrations in water at the point where meteoric waters enter the formation.

Another dating technique compares the ratio of ^{238}U to its daughter ^{234}U. Deviation from concentrations expected when these two isotopes are in secular equilibrium, may indicate travel from the formation in which the ^{238}U occurs. In these cases a good understanding of the mineralogy of the aquifer is necessary to account for isotope exchange and fractionation processes. This is often done by comparing the exchange of fractionation of stable isotopes (*e.g.*, ^{13}C when using ^{14}C).

3.4.2.1 Interaction with other parameters

The age of water is influenced by the hydrological parameters: water inflow rate, permeability, and water potential (hydraulic head). To interpret the data in some situations it is also necessary to know the mineralogy of the aquifer. To be able to interpret situations where two aquifers may have mixed and affected the measured age, the stratigraphy of the formation must also be understood. Work on age dating by isotopes cannot be done in isolation from these hydrologically critical parameters, but must be done as an integrated research program.

The instrumental parameter, isotope concentration, can be influenced by exchange between isotopes in solution and in the formation rock, and by differential sorption or desorption. The fission of uranium in the formation produces neutrons which may create active isotopes such as ^{14}C or ^{36}Cl, raising their concentrations. It is important that age dating by isotope techniques be integrated with the study of the mineralogy and stratigraphy of the formation.

It is useful to compare the ages derived from various isotopes. When done with consideration for the mineralogy of the formation, corrections can be made for deviations due to isotope exchange or differential processes.

3.4.2.2 Normal parameter range

Groundwater ages up to 100 years can be measured by tritium dating and up to 25,000 years using ^{14}C dating techniques. The $^{238}U/^{234}U$ dating technique can measure water ages up to 100,000 years, and ^{36}Cl can be used to date waters to 1,000,000 years.

3.4.2.3 Is this parameter site sensitive?

Rock formations vary in permeability, water potential, and extent. Thus, this parameter is site sensitive. Also, fractionation of isotopes due to various mechanisms in the hydrologic cycle requires calibration for waters of each hydrostratigraphic unit at a site. The $^{238}U/^{234}U$ technique is sensitive to uranium content of groundwater and the extent of rock-water interface. In all cases, calibration must be done for each hydrostratigraphic unit of the site since water of different units and ages sometimes mix. The ^{14}C method is sensitive to the presence of carbonate minerals since ^{14}C may exchange with ^{12}C and produce spuriously greater age.

3.4.2.4 Expected parameter variations during normal site operation

This is unknown, but the potential for variation in the direction of younger water is large in the near-repository region because of changes in permeability induced by human activities. Furthermore, human activities could alter the flow patterns leading to mixing of waters from different hydrostratigraphic units, consequently, causing difficulties in making accurate age determinations.

3.4.2.5 Parameter values that may signal trouble

While groundwater discharge rates upstream from the repository (as indicated by water age) may not have a direct effect on downstream flow, young age may indicate trouble when upstream and downstream rock formations are compared. One of the age-dating isotopes, tritium, has been introduced into the environment by atmospheric nuclear weapons tests at levels that were initially up to one hundred times greater than those produced by natural processes. This provides a clear signal of very young waters. In any case, the presence of tritium, with its twelve year half-life, may signify very young water (between 20 and 100 years since its precipitation) and consequent rapid flow rates or a short path. Since it is possible for *in situ* decay of uranium and thorium to generate tritium, this conclusion must be weighed against the occurrence of uranium and thorium in the formation.

3.4.2.6 What may happen if this parameter is not measured?

If water age is not determined, other means of measuring groundwater flow rates exist, but age dating of the water will increase the degree of confidence that can be placed in them.

3.4.3 Sorptive Capacity of Formation Rock

Rock around the repository site may sorb different radionuclides to varying degrees. The effect is to retard the release of radionuclides to the biosphere in varying degrees. Depending on values of sorptive capacity of fracture lining material and of backfill material, it is possible that the backfill will have the dominant effect on retardation of radionuclide leakage. Sorptive capacity should be measured during the site characterization phase.

3.4.3.1 Interaction with other parameters

These parameters will interact with groundwater chemistry. Temperature, complexing ions, pH, and Eh all affect the thermodynamics and kinetics of sorption.

3.4.3.2 Normal parameter range

A measure of sorptive capacities of minerals is the distribution coefficient, called K_d, R_d, or D in the literature. It is influenced by the particular combination of radionuclide sorbing mineral, and type and concentration of groundwater solutes. Expressed as the ratio of material sorbed per gram of mineral to material remaining per milliliter of solution, K_d can range from 0 to 70,000. A K_d of 0 means that no material is sorbed, while a K_d of 1000 means that over 99.9 percent has been sorbed. "The complexity of these interactions and sheer numbers of parameters and constituents which are important, necessitates the use of computers" (Serne and Relyea, 1982). Several computer codes have been developed which can be used or adapted to make predictions of sorption behavior. These include WATEQ, developed by the U.S. Geological Survey (Ball *et al.*, 1979), and EQ3/EQ6, developed at LLNL (Wolery, 1979).

3.4.3.3 Is this parameter site sensitive?

The sorptive capacity of tuff is expected to vary, even within a particular formation. Such features as lithophysae and vitrophyre are just the extreme examples of conditions affecting sorptive capacity. This parameter is site sensitive.

3.4.3.4 Expected parameter variations during normal site operation

Until radionuclides migrate beyond the backfill, this parameter will not change so that, in a narrow sense, it will not vary during normal occupation of the site. As radionuclides are released from the site, they will be sorbed by formation rock, using up the sorptive capacity. Those radionuclides that are up-stream will migrate further before they encounter unloaded material. Due to the temperature increase after emplacement of high level waste, it is expected that sorptive capacity, *per se*, will not change. However, the kinetics of sorption reactions will, so that sorption will occur more slowly. Dissolved radionuclides will migrate further into cooler sections of the formation before being sorbed.

3.4.3.5 Parameter values that may signal trouble

Again, the complexity of this question makes it impossible to give a quantitative answer at this time. Researchers are working on the problem. Sorptive capacity of formation rock is only one element in calculating the retarding effects of the rock formation. While high values of sorptive capacity are desirable, it is possible for greater fracture surface area or low rate of groundwater flow to compensate for low sorption values. A mineral with $K_d < 1$ will leave more radionuclide in solution than it adsorbs.

3.4.3.6 What may happen if this parameter is not measured?

If this parameter is not measured, accurate prediction of the migration rate of radionuclides in the far-field will not be possible.

3.4.4 Solubility of Radionuclides of Interest

Radionuclide solubilities have been studied in the laboratory and are well characterized.

Baes and Mesmer, 1976, provide a discussion, element by element, of radionuclide solubilities. Solubilities vary depending on temperature and the groundwater chemistry parameters: pH, Eh, and anion concentrations. There are three broad categories of radionuclides, based on their positions on the periodic table. The first category is iodine and cesium, which will be soluble under all natural conditions. However, iodine may be precipitated by properly chosen additions to backfill material. The second category is the alkaline earth materials, which in nuclear waste are represented mainly by barium, strontium, and radium. These will all be precipitated by the carbonates and sulfates present in groundwater or minerals; precipitation is influenced by pH. The third category is the transition metals, lanthanides, and actinides, many of which have several oxidation states. Each state has a different solubility, with the more oxidized states being more soluble. Although the near-field may be expected to have a relatively high Eh due to exposure to air, far-field conditions are expected to be such as to precipitate these radionuclides. In the case of plutonium, the reduction reaction is expected to take place on mineral surfaces. Even though the solution Eh can be oxidizing, the mineral may nonetheless precipitate it. Radionuclide solubility can be determined by calculation rather than *in situ* measurement.*

Another means of transportation of some radionuclides is by colloidal suspension. Many actinides and a few transition metals form hydroxide colloids under the appropriate conditions. Colloidal particles must be smaller than the fractures in rocks to pass through them. Colloidal particles may be aggregated into larger ones by the process of flocculation. Here the critical variables are particle size and surface charge. Particle size is a function of pH and radionuclide concentration. Flocculation is dependent on pH, ion types, and their concentration in groundwater. Flocculation can be determined by consulting literature and calculation, rather than *in situ* measurement.

3.4.4.1 Interaction with other parameters

Solubility of radionuclides is so strongly affected by groundwater chemistry and its aforementioned subparameters, that it can be said to be determined by them. Groundwater anions can greatly increase the solubility of many radionuclides by forming ionic complexes. Each of the many complexes which can form from these radionucides, and even just one type of anion, is considered a separate species for the purpose of determining equilibrium solubility. The interaction is complex. Solubilities are also affected by temperature, most solubilities varying directly with this parameter.

3.4.4.2 Normal parameter range

This is an extremely intricate issue. It must be answered for each radionuclide with reference to all groundwater constituents and, in some cases like that of iodine, with reference to other radionuclides. In principle, they can be predicted (given these data) using computer programs such as WATEQ (Ball *et al.*, 1979) and EQ3/EQ6 (Wolery, 1979).

3.4.4.3 Is this parameter site sensitive?

Since radionuclide solubility is strongly affected by the groundwater chemistry, which is site sensitive, it is also site sensitive.

3.4.4.4 Expected parameter variations buring normal site operation

The most important influence on the solubility of certain radionuclides that can occur during normal site occupation is the spill of anthropogenic organics in the repository. The most likely sources of such materials in a repository are decontaminating agents, drilling muds, rust removers, and detergents. Since their presence depends on the nature and extent of such spills and the thoroughness of cleanup, it presently is not possible to quantify this. Knowing the amount of such materials remaining in the repository after closure will be necessary to predict the effect on radionuclide solubility. Therefore, analyses of all such materials should be done and a record of their use, spills, and cleanup should be kept. After cleanup, and certainly before repository closure, accumulated water should be analyzed for these organics.

Radionuclide solubility will also vary, as previously discussed, due to temperature variations during the site operation and closure phases.

3.4.4.5 Parameter values that may signal trouble

The solubilities of most radionuclides depend on the chemistry of the groundwater. However, iodine and cesium, especially the latter, will have high solubilities under any conditions. Therefore, a record of the cesium loading of the waste should be kept. Iodine forms insoluble or slightly soluble salts with some of the transition metals, which will be among the other radionuclides present in the waste, so that its concentration in the waste must be compared with the concentration of the other radionuclides.

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*Most solubility studies have been done at 25°C. It is important to confirm predictions of solubilities by laboratory studies at temperatures expected in a repository.

3.4.4.6 What may happen if this parameter is not measured?

Without the capability of measuring this parameter, the transport of radionuclides cannot be predicted. The solubilities of radionuclides, with respect to each other and common groundwater constituents, are presently being investigated for the temperature and pressure ranges expected in repository environments. A number of computer codes are being tested and databases are being established that will lead to calculations of the expected concentrations of radionuclides if the concentrations of groundwater constituents and supply of radionuclides are known.

3.4.5 Volatility and Gaseous Diffusion of Radionuclide Chemical Species

In unsaturated highly porous rock, such as tuff, there exists a medium for the gas phase transport of radionuclides. Therefore, the volatility of various radionuclide compounds must be considered, along with the availability of other elements necessary for their formation and the thermodynamics of those reactions.

First among fission product radionuclides to be considered in this regard is xenon 129. This will be gaseous under all conceivable conditions in a repository, and can be considered the worst case example for gaseous diffusion of radionuclides. Its nine day half-life would render it unimportant except that it is the decay product of iodine 129, which has a 16 million year half-life. Iodine and some of its tin compounds will have considerable vapor pressures at repository temperatures and must also be considered as candidates for gaseous transport.

Diffusion rates will be determined by temperature, the pressure of void space gas, the molecular weight of volatile radionuclide species, rock porosity, and tortuosity. In principle, diffusion rates can be calculated from these data, except that possible adsorption reactions have not been studied. These include reactions between volatile radionuclides and surfaces of canisters, backfill, seals, formation rock, and infiltrating water. The diffusive transport of gaseous radionuclides is discussed in the Appendix.

As mentioned, iodine, both in elemental form and in the compound tin dichloride diiodide, is the radionuclide must likely to be transported in the gas phase. Tin is also a high-yield fission product radionuclide. The chlorine in tin dichloride diiodide will be available from infiltrating water. The creation of elemental iodine from its ionized forms is by endothermic reactions, but with the intense gamma radiation expected in the early years after emplacement this is not a limitation.

Bromine is also a fission product radionuclide which will have high volatility, both in elemental form and in tin compounds. Tin bromide-iodide compounds could form before groundwater comes in contact with the waste form. Since it is not an appreciable fission product, compounds containing chlorine will not form until after groundwater carrying chloride leaches into the canisters.

The fluorides of a number of radionuclides are volatile. These include antimony, ruthenium, molybdenum, and niobium fluorides. Since fluorine is not an appreciable fission product and fluoride occurs only in trace amounts in groundwaters, these are not expected to be important in the vapor phase transport of radionuclides.

The hydrides of antimony and tellurium boil at very low temperatures, but are not expected to form in the oxidizing environment of a repository.

Tritium is a gaseous fission product, significant levels of which may be present in high-level wastes if these wastes are fairly fresh. It diffuses readily through solids so that it will not occur in significant quantities in wastes that have been stored more than a few years after removal from a reactor. Its twelve-year half-life means that even for fresh wastes it is more of a hazard during site operation than after closure.

3.4.5.1 Interaction with other parameters

The formation of gaseous radionuclides is dependent on temperature, other energy inputs such as gamma and beta fluxes, and the chemical composition of infiltrating groundwater. The diffusion of gases is a function of temperature, pressure, and molecular weight. Adsorption of these gases is influenced by the chemical composition of the rock through which it diffuses.

3.4.5.2 Normal parameter range

All candidate radionuclides for gas-phase transport will have appreciable vapor pressures below their boiling points. Boiling point data (Table 16) give a relative ordering according to expected amount transported and the distance traveled.

For more detailed information about the vapor pressures of volatile compounds of radionuclides, consult the tabulation compiled by Strull (1947). For the diffusion coefficients of xenon in nitrogen, see Marrero and Mason (1972).

3.4.5.3 Is this parameter site sensitive?

Since the volatility of some radionuclides depends on their forming compounds with chemicals that may or may not be available in infiltrating groundwater, this parameter is site sensitive. Diffusion rates are dependent on the porosity and tortuosity of the repository rock, and are thus site sensitive.

3.4.5.4 Expected parameter variations during normal operation

The volatility of those radionuclides that may form compounds during operation is dependent on temperature. As the temperature of the repository rises due to the emplacement of high-level wastes, the volatility of those radionuclides will increase.

3.4.5.5 Parameter values which may signal trouble

The degree of trouble indicated by this parameter is inversely proportional to the absolute temperature of the boiling point for each volatile radionuclide species. Except for its relative scarcity in fission products, krypton would be more troublesome than xenon. Tin dichloride diiodide will be considerably less trouble, particularly if the repository temperature does not approach its boiling point.

Table 16. Boiling points of candidate radionuclides for gas-phase transport.

Radionuclide species	Formula	Boiling point [°C]
krypton	Kr	−152
xenon	Xe	−107
antimony hydride	SbH_3	−17
tellurium hydride	TeH_2	−2
molybdenum hexafluoride	MoF_6	35
tin bromide trichloride	$SnBrCl_3$	50
bromine	Br	59
tin dibromide dichloride	$SnBr_2Cl_2$	65
tin chloride tribromide	$SnBr_3Cl$	73
tin tetrachloride	$SnCl_4$	114
antimony pentafluoride	SbF_5	149
molybdenum oxytetrafluoride	$MoOF_4$	180
iodine	I_2	184
tin tetrabromide	$SnBr_4$	202
tin dibromide diiodide	$SnBr_2I_2$	225
niobium pentafluoride	NbF_5	236
ruthenium pentafluoride	RuF_5	250
niobium pentachloride	$NbCl_5$	254
tin dichloride diiodide	$SnCl_2I_2$	297

3.4.5.6 What if this parameter is not measured?

The volatility data needed for computer models of gaseous diffusion already exist in tabular form. However, reaction mechanisms, thermodynamics, and kinetics for the formation of volatile radionuclide species and their adsorption by rock surfaces must be studied in the laboratory. Without these studies, significant factors in gaseous transport of radionuclides will remain unknown.

3.4.6 Canister and Support System Corrosion

The rate of canister corrosion is a critical parameter and should be measured *in situ* using test canisters during the periods of site characterization and repository operation, and, after closure, in a simulated environment. Moisture and temperature at the canister surface are the major determinants of corrosion rate, and themselves are critical parameters because of this. The groundwater components, chloride and magnesium, have been shown to enhance the corrosion of steel, so that their concentrations are also critical parameters.

The corrosion of support structures must also be considered. These include rock bolts, plates, beams and chain link fencing used to minimize wall and ceiling movements in shafts and drifts. These will be exposed to the same chemical environment as the canisters, though the radiological effects will probably be attenuated. Since they serve a different function, being under stress, they may be made from different materials. Support structure corrosion can be treated the same as canister corrosion, except that it is most important during site operation.

Maintaining canister integrity for 300 to 1,000 years or longer has been considered to ensure that only a relatively small quantity of long-lived radionuclides will remain when the canister finally is breached.

The length of time that canister integrity is maintained is important, even above and beyond this. The rate of waste form devitrification (if it is a glass) and leaching will depend strongly on temperature. Devitrification can begin as soon as the waste form has solidified and is sufficiently heated. Leaching processes will begin when the canister is breached and water reaches the waste. The leaching rate will vary directly with temperature. Repository temperature is itself a function of time following the emplacement of waste. With canisters intended to last through the period of maximum temperature, temperature will be declining monotonically when they breach. All other things being equal, the rate of leaching will decline slowly with time. Since exposed surface area of the waste form may increase with time, leaching rate as a function of time is a complex problem.

During the period of repository construction and operation, the repository will be filled with atmospheric air, and all materials in it will be exposed to abundant free oxygen. The pores in the backfill will be filled with air when it is emplaced, and some atmospheric oxygen will probably penetrate into the rock surrounding the repository. In all cases, the presence of oxygen will effectively increase Eh (oxidation potential), and oxygen in the backfill will accelerate canister and support system corrosion.

Due to the intense gamma radiation of high-level wastes, several significant radiolytic reactions may occur. Several sets of possible atmospheric conditions inside the canister emplacement borehole need to be addressed to reflect the possible presence and absence of water and oxygen.

The following are expected chemical conditions after nuclear waste emplacement in the canister borehole. It is assumed that the borehole will initially be dry but filled with air, either by itself or with some dry, porous, granular material containing some fraction of air. Gamma radiation breaks up nitrogen and oxygen molecules to create their respective radicals and ions. Some recombine to form nitrogen oxides. If the atmosphere contains only nitrogen, then no nitrogen oxides will form. The formation of the nitrogen oxides is a highly endothermic reaction, with the energy supplied by the gamma radiation.

Eventually water will seep into the very-near-field, most likely as steam in its earliest appearance. If nitrogen oxides have formed already, these will combine with the water vapor to form nitric acid. After water is present, hydrogen, oxygen, and hydroxyl radicals and ions will also be formed by radiolysis. If the borehole has been anoxic, then nitrogen radicals and ions will react with water molecules and its radical products to form nitric acid and hydrogen. In the anoxic borehole, nitrogen oxides will not form until after steam reaches the region of strong gamma activity.

While nitric acid will corrode some metals, it will passivate others. Nitric acid can also be expected to increase the solubility of many radionuclides. Hydrogen gas can embrittle some metals. Nitric acid may corrode the steel canister and hydrogen may cause hydrogen embrittlement of the steel. Support system material exposed to the nitric acid and hydrogen may also be affected. The rates of nitric acid or hydrogen formation, and the total amounts formed, depend on the radiation level and the fugacities of oxygen or water in irradiated spaces.

The fugacity[*] of oxygen in the backfill is a critical subparameter. It is presumed that the oxygen in the repository will rapidly be removed by reaction with the crushed basalt in the backfill after the repository is sealed. This needs to be confirmed by measuring the oxygen fugacity near test canisters, employing suitable *in situ* instrumentation.

Hydrogen fugacity is a critical, dependent, subparameter. Hydrogen embrittlement of some candidate canister materials is possible. Hydrogen in the repository atmosphere will make it a reducing environment, and will tend to retard canister corrosion. Which of these two effects is dominant will depend on engineering decisions about waste loading and backfill moisture (Stahl and Miller, 1983).

The initial water fugacity of the repository may depend on engineering decisions regarding backfill material and its water content. Water fugacity also influences backfill behavior. Some of the candidate backfill materials swell as they absorb water. It is conceivable that, in a confined space, the swelling could lead to pressure which causes the collapse of canisters or the rupture of seals. Relatively simple design features can eliminate this problem. The behavior of backfill material with respect to water fugacity should be the subject of pilot studies.

When moisture penetrates the backfill and contacts the canister, corrosion will begin. After the canister has been breached, the water in the backfill will contact the waste form and leach radionuclides from it. Thus, rehydration of the backfill will strongly influence the processes of canister corrosion and waste form leaching. The fugacity of water or moisture profile in the backfill around at least some canisters must be monitored. Presumably, this will begin with some test canisters emplaced early during site characterization.

3.4.6.1 Interaction with other parameters

Canister and support system corrosion is a variable that is dependent on five other variables: temperature, the fugacities of oxygen and water, groundwater flow rate, and groundwater chemistry. Corrosion of steel is essentially the oxidation of iron, so that the activity of oxygen has a strong influence. This reaction is mediated and catalyzed by liquid water. In addition, chloride ions attack many stainless steels and the oxidation product by complexing with iron ions. Oxygen is used up by the corrosion reaction so that the rate at which oxygen is supplied to the metal surface is also important in determining the rate of corrosion. The oxygen supply rate is a function of oxygen fugacity and groundwater flow rate. Interaction of corrosion with temperature and groundwater chemistry are discussed in Sections 3.1.6 and 3.4.1, respectively.

3.4.6.2 Normal parameter range

The reference design for the waste canister assumed by DOE for a repository in the unsaturated zone is made of 304L stainless steel with walls 1.0 cm thick (DOE, 1984, Section 6.4.2.1.1). In low-salinity aerated water at near-neutral pH, the corrosion rate of 304L stainless steel was found to be less than 2.5×10^{-4} cm/yr. In tests using natural water taken from a tuff formation, kept at pressure to maintain a temperature of 105°C, and exposing the metal to 3×10^5 rad/h, the corrosion rate was less than 3.7×10^{-5} cm/yr (DOE, 1984, Section 6.4.2.2.1).

There are two aspects to measuring water fugacity. It is necessary to detect the presence of liquid water. The presence of liquid water defines the maximum fugacity of water that can exist at the given temperature and pressure. Lower values of water fugacity also must be monitored within the backfill. The minimum value of water fugacity at any given temperature will be that of the nominally dry backfill materials. This may be one or two-tenths the fugacity of liquid water. Values of water fugacity between these values must be measured *in situ*. These values will vary with temperature and pressure.

Saturation ratio is equivalent to water fugacity. This is fugacity divided by that of pure liquid water at the given temperature and pressure. The range of saturation ratio that needs to be determined will be between about 0.1 to 1.0 at any temperature and pressure.

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[*] Fugacity is a measure of the chemical potential of substance, expressed in units of pressure. In an ideal gas mixture, the fugacity of a gas is equal to its partial pressure. Fugacity is well defined, even if a vapor phase is not present.

3.4.6.3 Is this parameter site sensitive?

Canister and support system corrosion will be dependent on the amount of groundwater infiltration and the groundwater composition. Thus, it is site sensitive.

3.4.6.4 Expected parameter variations during normal site operation

The determining subparameter, water fugacity, may be affected by changes in rock permeability due to repository development. Some areas may experience a decline as water is channeled to other areas which experience an increase. Oxygen fugacity will be 0.21 bar as long as the workings are open to the atmosphere, but it will be reduced in areas where backfill has been emplaced or purged with an inert atmosphere. With respect to factors affecting corrosion rate, groundwater chemistry is not expected to vary greatly.

3.4.6.5 Parameter values that may signal trouble

Corrosion rate is dependent on, among other factors, the metal(s) used for the canister and support system components. This issue is best resolved by lab studies of candidate alloys under the conditions expected at candidate sites.

3.4.6.6 What may happen if this parameter is not measured?

If corrosion rates are not measured, nor attempts made to calculate them, it will be impossible to predict when radionuclides will begin leaching from the waste form. This is a step in the process of leakage from waste form to the biosphere, which is important for shorter-lived radionuclides that might be released due to early canister corrosion.

Without knowledge of support system corrosion rates, it will be difficult to engineer a structurally sound repository capable of providing a safe working environment and a reliable repository system over the operating and retrievability periods.

3.4.7 Radionuclide Leakage Rate

Radionuclide leakage through the repository formation, or rather its delay, is the rationale for the effort of nuclear waste storage. Monitoring leakage will provide the proof for all previous measurements, designs, and calculations. It can be done directly during site operations and after closure by taking water samples from monitoring wells bored at significant locations in the repository formation and analyzing the samples for radionuclides. They data combined with those from hydrologic studies will allow future generations to calculate the direction and velocity of the plume of radionuclides leaking from the repository, and estimate when they will reach the biosphere.

If liquid water is not present, radionuclides may first be transported in vapor phase, as discussed in Section 3.4.5, Volatility and Gaseous Diffusion of Radionuclide Chemical Species, and in the Appendix. Under such conditions, certain radionuclide chemical species may be carried to regions of the formation where liquid water is percolating downward. These species may then be carried by this water down to the saturated zone.

This parameter is a function of many others. Calculable influences include the exposed surface area of the waste form, radionuclide inventory, radionuclide solubility, temperature, water fugacity, and groundwater flow rates, all at the time of canister breaching and afterwards. Incalculable influences are: the geometry of corrosion of the canister, its variation among canisters, and its variation over time.

The rate of radionuclide leaching from the canister affects the rate of loading of the backfill.

There are two issues to be considered here. The first is the rate of travel of the front of the plume of leaking radionuclides. Determining this will give the time scale necessary for decision and action. The second issue is the steady state concentration of radionuclides in the plume. This gives a measure of the potential hazard when the plume reaches the biosphere.

3.4.7.1 Interaction with other parameters

The radionuclide leakage rate from a canister will be a function of radionuclide volatility, radionuclide solubility, temperature, groundwater flow rates and velocities, groundwater chemistry and temperature. It is the input term for backfill and seal leakage rates.

Radionuclide leakage through the formation has as an input term the seal leakage output term. Leakage through the formation is influenced by groundwater flow rates, groundwater chemistry, radionuclide solubility, radionuclide volatility, the sorptive capacity of the formation rock and temperature.

3.4.7.2 Normal parameter range

An important parameter which influences leaching rate is the exposed surface area of the waste form, which depends on engineering decisions not yet made, namely on the waste form itself. Laboratory simulation is the best means of studying leach rate.

The normal range of radionuclide leakage rate from the formation is influenced by many other parameters, some of which are based on engineering decisions not yet made. It is not possible to give a range at this time.

3.4.7.3 Is this parameter site sensitive?

Site-dependent variables affecting radionuclide leakage through the repository formation include groundwater flow rate, groundwater chemistry, fracture permeability, and the sorptive capacity of fracture lining material. Radionuclide leakage through the formation is thus site sensitive.

3.4.7.4 Expected parameter variations during normal site operation

Although the intent of repository design is to prevent leakage before closure, it is possible that corrosion of early placed canisters will be severe enough that leakage will begin during the operations phase. This problem can be obviated by laboratory and pilot studies of canister corrosion.

Radionuclide leakage through the repository formation will be influenced by the heating of the formation as thermal energy from the waste diffuses into it. At higher temperature the radionuclides will be more soluble and the kinetics of sorption will be less favorable. Thus, radionuclides can be expected to travel farther in the formation before they are sorbed. Any computer model of radionuclide migration through the formation must take into account the rise in temperature.

3.4.7.5 Parameter values that may signal trouble

The leakage rate from the canister is the supply term for backfill leakage calculations. Leakage rates should be determined by computer modeling and physical simulation. Simulations using exposed waste in pilot facilities can be used to determine modeling parameters.

Radionuclides leaking through a rock formation must travel distances on the order of 10 kilometers, and should take at least 10,000 years to do so. This is an average rate of 1.0 meter per year as a rough estimate of the maximum allowable rate for the front of any radionuclide plume migrating through the formation. Maximum permissible concentrations of radionuclides in water in the biosphere are established by government regulation and may change in the future.

3.4.7.6 What may happen if this parameter is not measured?

If radionuclide leakage from the canister cannot be determined, a critical source term is unavailable for calculating the radionuclide supply to mechanisms further along the escape path. This parameter is important to any modeling study.

If the rate of radionuclide leakage through the repository formation is not measured, then prediction of the date at which radionuclides reach the biosphere will be dependent on computer modeling. A thorough understanding of potential radionuclide leakage rates must include computer models using worst-case parameter values measured during testing. While computer modeling can, in principle, produce accurate results, it is susceptible to systematic errors due to human oversight. Monitoring of radionuclide migration can serve to confirm such predictions, and provide warning if they are incorrect.

3.4.8 Seal and Backfill Leakage

There are many configurations of seals and backfills that may be considered. Models of various combinations of physical layouts can be used to determine overall leakage. Data on leakage through seals and backfill can be obtained from laboratory and pilot studies during the site characterization phase. Actually, measurements of leakage out of the repository may be done with monitoring wells drilled at selected points in the far field during the operations and closure phases. Water samples taken from these wells would be analyzed for the various expected radionuclides. Since the site is expected to be operated for fifty years, leakage from sections filled earlier in the operation is an important consideration, not only as a pilot model for overall leakage, but for the health and safety of repository personnel. Before emplacement of seals and closure, backfill leakage can be monitored by taking samples and by using remote radiation detectors.

Although leakage through the backfill can be modeled with a pilot study, *in situ* measurements are also possible. Placement of tracers and detectors in the backfill will make it possible to monitor groundwater flow, even before release of radionuclides from breached canisters.

3.4.8.1 Interaction with other parameters

Backfill leakage rate is a function of groundwater flow rate, radionuclide leakage rate from the canister, and groundwater chemistry, backfill chemistry, backfill mechanical properties, and temperature. Seal leakage rate is a function of groundwater flow rate, properties of seal material, and backfill leakage rate.

3.4.8.2 Normal parameter range

Backfill and seal leakage are the functions of other parameters which will be fixed by engineering decisions, and should be determined by modeling.

3.4.8.3 Is this parameter site sensitive?

Backfill and seal leakage rates are a function of groundwater flow rate and groundwater chemistry, which are site dependent.

3.4.8.4 Expected parameter variations during normal site operation

Leakage rates are not determinable at this time. This parameter is critical after site closure. Seal and backfill materials should be tested in laboratory and *in situ* situations for a variety of thermal conditions, groundwater chemistries, and flow rates.

3.4.8.5 Parameter values that may signal trouble

Values for backfill and seal leakage rates will be fixed by engineering decisions not yet made and are necessary inputs for rock formation leakage calculations. Therefore, they should be determined by computer modeling and physical simulation during the design process.

3.4.8.6 What may happen if this parameter is not measured?

If this parameter cannot be determined, a critical rate in the overall repository flow pattern will be unavailable for calculation of radionuclide supply to mechanisms further along the flow path. It is important to any modeling study.

4.0 CONCLUSIONS

Identification of critical parameters and assignment of priorities to them show that certain parameters are prominent in specific phases of a repository's evolution. Of greatest concern in the site characterization phase is establishing an understanding of the geologic setting, especially the depth, thickness, orientation, and lateral continuity of hydrostratigraphic units encompassing and bounding the proposed repository rock mass. An understanding of the hydrologic characteristics of these hydrostratigraphic units is also of principal concern during the site characterization phase, with monitoring of these parameters continuing into subsequent phases. Measurements of the age of water, and the sorptive capacity of rock matrix and fracture lining materials are geochemical parameters of primary importance during the site characterization phase. These are closely followed in importance by measurements to determine: groundwater chemistry; solubility, volatility and gaseous diffusion of radionuclide species of interest; and canister and support system corrosion rates. The canister corrosion tests should be started during the site characterization phase, and long-term observations should be conducted throughout the entire repository sequence. Characterizating the lithophysal, fracture, thermal, thermomechanical, and mechanical properties of the rock mass also has a high priority during site characterization.

During the site construction phase, deformations and displacement, *in situ* stress changes, and induced fracturing will be of principal concern as the underground construction progresses through the rock mass. As the construction proceeds, new openings will provide accessibility for additional measurements of important critical parameters that may vary through the rock mass, such as: water potential, degree of water saturation of the rock, age of water, geologic variables, fracture properties, rock strength, variations in virgin *in situ* stress, variations in rock modulus and Poisson's ratio, and tectonic factors.

The highest-priority critical parameters during the site operation phase include those concerned with the response of the rock mass and hydrologic system to thermal effects from the introduction of radioactive waste. High priority critical parameters requiring measurement and long-term monitoring systems, installed during operations and extending into (and in some cases beyond) the closure and decommissioning phase of the repository, include those parameter concerned with radionuclide leakage and the effectiveness of backfill and sealing systems.

Several geologic parameters, such as faulting, folding, and erosion rate, are not directly measurable by instrumentation systems, but may be determined indirectly by surface and/or subsurface geophysical techniques. Similarly, not all hydrologic parameters are directly measurable, but rely on interpretation of measurements of specific hydrologic properties of the rock mass.

In several cases, parameters will be measured initially in test facilities that will begin operation during the site characterization phase. The most important tests will monitor the performance of canisters, backfill and seals, and the hydro-thermo-mechanical response of the rock mass to the introduction of the waste. These measurements and long-term monitoring will subsequently be extended to the actual repository locations as canisters are emplaced and as the full-scale sealing systems are established.

It is important to keep in mind that the relative ranking of closely spaced (in importance) parameters is only approximate, and can change significantly depending on site-specific considerations and increased understanding of each parameter's importance.

Even though the rank ordering is somewhat subjective and can change with future information, the magnitude of each change will probably not be great. The exact priority of each parameter is considered less important than having the critical parameters clearly defined.

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REFERENCES

Apps, J.A., C.L. Carnahan, P.C. Lightner, M.C. Michel, D. Perry, R.J. Silva, O. Weres, and A.F. White (1983), *Status of Geochemical Problems Relating to the Burial of High-Level Radioactive Waste, 1982,* prepared by Lawrence Berkeley Laboratory for the U.S. Nuclear Regulatory Commission, NUREG/CR-3062.

Apps, J.A., T. Doe, B. Doty, S. Doty, R. Galbraith, A. Kearns, B. Kohrt, J.C.S. Long, A.P. Monroe, T.N. Narasimhan, P.H. Nelson, C.R. Wilson, and P.A. Witherspoon (1979), *Geohydrologic Studies for Nuclear Waste Disposal at the Hanford Reservation,* Lawrence Berkeley Laboratory, Berkeley, California, LBL-8764.

Baes, C.F., and R.E. Mesmer (1976), *The Hydrolysis of Cations,* John Wiley and Sons, New York.

Ball, J.W., E.A. Jenne, and D.K. Nordstrom (1979), "WATEQ2-A Computerized Chemical Model for Trace and Major Element Speciation and Mineral Equilibria in Natural Waters," *Chemical Modeling of Aqueous Systems,* ACS Symposium Series 93, pp. 815–835, American Chemical Society, Washington, D.C.

Bass Becking, L.G.M., I.R. Kaplan, and D. Moore (1960), "Limits of the Natural Environment in Terms of pH and Oxidation-Reduction Potentials," *Journal of Geology,* Vol. 68, No. 3, pp. 243–284.

Benson, S.M., (1984), *Analysis of Injection Tests in Liquid-Dominated Geothermal Reservoirs,* M.S. Thesis, University of California, Berkeley, California. Lawrence Berkeley Laboratory, Berkeley, California, LBL-17953,

Benson, S.M., and G.S. Bodvarsson (1982), *Nonisothermal Effects During Injection and Falloff Tests,* Society of Petroleum Engineers paper SPE-11137, presented at the 57th Annual Meeting of the Society of Petroleum Engineers, New Orleans, Louisiana, September 1982.

Binnall, E.P., H.A. Wollenberg, S.M. Benson, L. Tsao, O. Weres, A.L. Ramirez, and G.A. Armantrout (1985), *Critical Parameters for a High-Level Waste Repository, Volume 1: Basalt,* prepared by Lawrence Berkeley Laboratory and Lawrence Livermore National Laboratory for the U.S. Nuclear Regulatory Commission, NUREG/CR-4161, Vol. 1. Lawrence Livermore National Laboratory, Livermore, California, UCID-20092, Vol. 1.

Binnall, E., and M. McEvoy (1985), *Assessment of Thermocouple Temperature Measurements During In Situ Heater Experiments at Stripa, Sweden,* prepared by Lawrence Berkeley Laboratory for the U.S. Department of Energy, LBL-1260, SAC-54.

Carr, W.J., (1974), *Summary of Tectonic and Structural Evidence for Stress Orientation at the Nevada Test Site,* U.S. Geological Survey, open-file report, OF-74-176.

Chan, T., E. Binnall, P. Nelson, R. Stolzman, O. Wan, C. Weaver, K. Ang, J. Braley, and M. McEvoy (1980), *Thermal and Thermomechanical Data from In Situ Heater Experiments at Stripa, Sweden,* Lawrence Berkeley Laboratory, Berkeley, California, LBL-11477, SAC-29.

Cook, N.G.W. and M. Hood (1978), *Full-Scale and Time-Scale Heating Experiments at Stripa: Preliminary Results,* prepared by Lawrence Berkeley Laboratory for the U.S. Department of Energy, LBL-7072, SAC-11.

Constanz, J., (1983), "Laboratory Analysis of Water Retention in the Unsaturated Zone Materials at High Temperature," in *Role of the Unsaturated Zone In Radioactive and Hazardous Waste Disposal*, J.W. Mercer, P.S.C. Rao and I.W. Marine, Eds., Ann Arbor Science, Ann Arbor, Michigan, pp. 147–164.

DOE (1984), *Draft Environmental Assessment, Yucca Mountain Site, Nevada Research and Development Area, Nevada*, U.S. Department of Energy, Office of Civilian Radioactive Waste Management, DOE/RW-0012, December 1984.

Drost, W., D. Klotz, A. Koch, H. Moser, F. Neumaier, and W. Rauert (1968), *Point Dilution Methods of Investigating Groundwater Flow by Means of Radioisotopes.* Water Resources Research, 4(1), pp. 125–146.

Elzeftawy, A., and K. Cartwright (1981), "Evaluating the Saturated and Unsaturated Hydraulic Conductivity of Soils," in *Permeability and Groundwater Contaminant Transport*, ASTM STP 746, T.F. Zimmie and C.O. Riggs, Eds., American Society for Testing and Materials, 1981, pp. 168–181.

Evans, D.D. (1983), *Unsaturated Flow and Transport Through Fractured Rock — Related to High-Level Waste Repositories*, prepared for the U.S. Nuclear Regulatory Commission, NUREG/CR-3208.

Fernandez, J.A. and M.D. Freshley (1984), *Repository Sealing Concepts for the Nevada Waste Storage Investigations Project*, prepared by Sandia National Laboratories for the U.S. Department of Energy, SAND83-1778, Sandia National Laboratories, Albuquerque, New Mexico.

Freeze, A.R. and J.A. Cherry (1979), *Groundwater*, Prentice-Hall, Englewood Cliffs, New Jersey.

Goodman, R.E. (1980), *Introduction to Rock Mechanics*, John Wiley and Sons.

Grizak, G.E., W.F. Merritt, and D.W. Williams (1977). *A Fluoride Borehole Dilution Apparatus for Ground Water Velocity Measurements*, Canadian Geotechnical Journal, 14, pp. 554–561.

Guven, O., R.W. Falta, F.J. Molz, and J.G. Melville (1985). *Analysis and Interpretation of Single-Well Tracer Tests in Stratified Aquifers*, Water Resources Research, Vol. 21, No. 5, pp. 676–684, May 1985.

Hamilton, J.M., D.E. Daniel, and R.E. Olson (1981), "Measurement of Hydraulic Conductivity of Partially Saturated Soils", in *Permeability and Groundwater Contaminant Transport*, ASTM STP 746, T.F. Zimmie and C.O. Riggs, Eds., American Society for Testing and Materials, pp. 182–196.

CRC Handbook of Chemistry and Physics, 53rd Edition (1972), CRC Press.

Hillel, D. (1980), *Applications of Soil Physics*, Academic Press, New York, New York.

Hillel, D. (1980a), *Fundamentals of Soil Physics*, Academic Press, New York, New York.

Jaeger, J.C. and N.G.W. Cook (1979), *Fundamentals of Rock Mechanics*, Third Edition, Chapman and Hall.

Javendal, I. (1983), *Field Determination of the Hydrologic Properties and Parameters that Control the Vertical Component of Groundwater Movement*, Lawrence Berkeley Laboratory Report, LBL-15050, University of California, Berkeley, California.

Johnstone, J.K., R.R. Peters, and P.F. Gnirk (1984), *Unit Evaluation at Yucca Mountain, Nevada Test Site: Summary Report and Recommendations*, prepared by Sandia National Laboratories for the U.S. Department of Energy, SAND83-0372, June 1984.

Klasi, M.L., W.C. McClain, and T. Brandshaug (1982), *Far-Field Thermal Analysis of a Spent Fuel Repository in Tuff,* prepared by RE/SPEC Inc. and Sandia National Laboratories for the U.S. Department of Energy, SAND81-7209, July 1982.

Klasi, M.L., J.E. Russell, W.C. McClain, and T. Brandshaug (1982a), *Far-Field Thermal Analysis of a High Level Waste Repository in Tuff,* prepared by RE/SPEC Inc. and Sandia National Laboratories for the U.S. Department of Energy, SAND81-7210, July 1982.

Lappin, A.R. (1980), *Preliminary Thermal Expansion Screening Data for Tuffs,* prepared by Sandia National Laboratories for the U.S. Department of Energy, SAND78-1147, March 1980.

Long, J.C. (1983), *Investigation of Equivalent Porous Medium Permeability in Networks of Discontinuous Fractures,* Lawrence Berkeley Laboratory, Berkeley, California, LBL-16259.

Marrero, T.R. and E.A. Mason (1972), "Gaseous Diffusion Coefficients," *Journal of Physical and Chemical Reference Data,* Vol. 1, No. 1.

Montazer, P.M. (1982), *Permeability of Unsaturated, Fractured Metamorphic Rocks Near an Underground Opening,* Ph.D Thesis, Colorado School of Mines, Denver, Colorado.

Montazer, P., and W.E. Wilson (1984), *Conceptual Hydrologic Model of Flow in the Unsaturated Zone, Yucca Mountain, Nevada,* U.S. Geological Survey, Water Resources Report 84-4345, Lakewood, Colorado.

Montazer, P., D.P. Hammermeister, and M.S. Whitfield (1985), *Drilling, Instrumentation, and Preliminary Testing Results of Borehole USW UZ-1 Penetrating Thick Unsaturated Tuffs, Yucca Mountain, Nye County, Nevada,* Water Resources Investigation Series, in preparation, 1985.

Morris, D.A., and A.I. Johnson (1967), *Summary of Hydrologic and Physical Properties of Rock and Soil Materials, as Analyzed by the Hydrologic Laboratory of the U.S. Geological Survey 1948–1960,* U.S. Geological Survey Water-Supply Paper, 1839-D.

Morrison, R.D. (1983), *Groundwater Monitoring Technology,* TIMCO MFG., INC. Praire Du Sac, Wisconsin.

Mualem, Y. (1976), *A New Model for Predicting the Hydraulic Conductivity of Unsaturated Porous Media,* Water Resources Research 12(3), pp. 513–522.

Nelson, P.H., R. Rachiele, and A. Smith (1980), *The Effect of Radon Transport in Groundwater Upon Gamma Ray Borehole Logs,* Lawrence Berkeley Laboratory, Berkeley, California, LBL-11180.

Nelson, P.H., R. Rachiele, J.S. Remer, and H. Carlsson (1981), *Water Inflow into Boreholes During the Stripa Heater Experiments,* Lawrence Berkeley Laboratory, Berkeley, California, LBL-12574, SAC-35.

Olson, R.E., and D.E. Daniel (1981), "Measurement of the Hydraulic Conductivity of Fine-Grained Soils," in *Permeability and Groundwater Contaminant Transport,* ASTM STP 746, T.F. Zimmie and C.O. Riggs, Eds, American Society for Testing and Materials, pp. 18–64.

O'Neal, W.C., L.B. Ballou, D.W. Gregg, and E.W. Russell (1984), "Nuclear Waste Package Design for the Vadose Zone in Tuff," *Waste Management '84, Proceedings of the Symposium on Waste Management at Tucson, Arizona, March 11–15, 1984,* R.G. Post (Ed), Vol. 1, pp. 547–551.

Paulsson, B.N.P. (1983), *Seismic Velocities and Attenuation in a Heated Underground Granitic Repository, Vols. I and II,* Ph.D Thesis, University of California, Berkeley, California. Lawrence Berkeley Laboratory report LBL-16346, SAC-51.

Paulsson, B.N.P., M.S. King, and R. Rachiele (1980), *Ultrasonic and Acoustic Emission Results from the Stripa Heater Experiments,* Lawrence Berkeley Laboratory, Berkeley, California, LBL-10975, SAC-32.

Peck, A.J., and R.H. Rabbidge (1969), *Design and Preformance of an Osmotic Tensiometer for Measuring Capillary Potential,* Soil Science Society of America Proceedings, 33:196–202.

Peters, R.R. (1983), *Thermal Response to Emplacement of Nuclear Waste in Long, Horizontal Boreholes,* prepared by Sandia National Laboratories for the U.S. Department of Energy, SAND82-2497, April 1983.

Peters, R.R., E.A. Klavetter, I.J. Hall, S.C. Blair, P.R. Heller, G.W. Gee (1984), *Fracture and Matrix Hydrologic Charactersitics of Tuffaceous Materials from Yucca Mountain, Nye County, Nevada,* prepared by Sandia National Laboratories for the U.S. Department of Energy, SAND84-1471.

Pratt, H.R., W.A. Hustrulid, and D.E. Stephenson (1978), *Earthquake Damage to Underground Facilities,* Savannah River Laboratory Report DP-1513.

Price, R.H., K.G. Nimick, and J.A. Zirzow (1982), *Uniaxial and Triaxial Compression Test Series on Topopah Spring Tuff,* prepared by Sandia National Laboratories for the U.S. Department of Energy, SAND 82-1723, October 1982.

Price, R.H., S.J. Spence, and A.K. Jones (1984), *Uniaxial Compression Test Series on Topopah Spring Tuff from USW GU-3, Yucca Mountain, Southern Nevada,* prepared by Sandia National Laboratories for the U.S. Department of Energy, SAND83-1646, February 1984.

Pruess, K., Y.W. Tsang, and J.S.Y. Wang (1984), *Numerical Studies of Fluid and Heat Flow Near High-Level Nuclear Waste Packages Emplaced in Partially Saturated Fractured Tuff,* Lawrence Berkeley Laboratory Report LBL-18552, University of California, Berkeley, California.

RHO, Rockwell Hanford Operations (1982), *Site Characterization Report for the Basalt Waste Isolation Project,* prepared for the U.S. Department of Energy, DOE/RL 82-3.

Rice, W.A. (1984), *Preliminary Two-Dimensional Regional Hydrologic Model of the Nevada Test Site and Vicinity,* prepared by Sandia National Laboratories for the U.S. Department of Energy, SAND83-7466, Albuquerque, New Mexico.

Rogue, F., and E.P. Binnall (1983), *Reliability of Geotechnical, Environmental, and Radiological Instrumentation in Nuclear Waste Repositories,* Lawrence Livermore National Laboratory, Livermore, California, UCID-19467, prepared for the U.S. Nuclear Regulatory Commission, NUREG/CR-3494.

Rosholt, J.N. and D.C. Noble (1969), *Loss of Uranium from Crystallized Silicic Volcanic Rocks, Earth and Planet,* Science Letters, Vol. 6, No.4, pp. 268–270.

Ross, B. (1984), *A Conceptual Model of Deep Unsaturated Zones With Negligible Recharge,* Water Resources Research, Vol. 20, No. 11, pp. 1627–1629.

Rulon, J., and G.S. Bodvarsson (1985), *Preliminary Numerical Simulations of Groundwater Flow in the Unsaturated Zone, Yucca Mountain, Nevada,* Lawrence Berkeley Laboratory Report LBL-20553, University of California, Berkeley, California.

Sass, J.H., and A.H. Lachenbruch (1982), *Preliminary Interpretation of Thermal Data from the Nevada Test Site,* U.S. Geological Survey Report USGS-OFR-82-973, Denver, Colorado.

Scheidegger, A.E. (1974), *The Physics of Flow Through Porous Media,* University of Toronto Press, Toronto, Canada. Third Edition.

Scott, R.B., R.W. Spengler, S. Diehl, A.R. Lappin, and M.P. Chornak (1983), "Geologic Character of Tuffs in the Unsaturated Zone at Yucca Mountain, Southern Nevada" in *Role of the Unsaturated Zone In Radioactive and Hazardous Waste Disposal,* J.W. Mercer, P.S.C. Rao, and I.W. Marine, Eds. Ann Arbor Science, Ann Arbor, Michigan, pp. 289–337.

Serne, R.J., and J.F. Relyea (1982), *The Status of Radionuclide Sorption-Desorption Studies Performed by the WRIT Program,* Battelle Pacific Northwest Laboratories, PNL-3997, UC-70, April 1982.

Sinnock, S., Y.T. Lin, and J.P. Brannen (1984), *Preliminary Bounds on the Expected Postclosure Performance of the Yucca Mountain Repository Site, Southern Nevada.* prepared by Sandia National Laboratories for the U.S. Department of Energy, SAND84-1492, Albuquerque, New Mexico.

Smith, G.V., T.S. Pink, J.R. Lawrence, L.A. Woodward, K. Keil, and A.R. Lappin (1981), *Preliminary Survey of Tuff Distribution in Esmeralda, Nye, and Lincoln Counties, Nevada,* prepared by Sandia National Laboratories for the U.S. Department of Energy, SAND 78-1839.

Sosman, R.B., (1985), *The Phases of Silica,* Rutgers University Press, New Brunswick, New Jersey.

Spaulding, W.G., S.W. Robinson, and F.L. Paillet (1984), *Preliminary Assessment of Climatic Change During Late Wisconsin Time, Southern Great Basin and Vicinity, Arizona, California, and Nevada.* U.S. Geological Survey, Water Resources Investigations Report 84-4328, Denver, Colorado.

St. John, C.M. (1985), *Thermal Analysis of Spent Fuel Disposal in Vertical Emplacement Boreholes in a Welded Tuff Repository,* prepared by Agbabian Associates and Sandia National Laboratories for the U.S. Department of Energy, SAND84-7207, November, 1985.

Stahl, D., and N.E. Miller (1983), *Long-Term Performance of Materials Used for High-Level Waste Packaging,* prepared for the U.S. Nuclear Regulatory Commission, NUREG/CR-3427, Vol. 2.

Strull, D.R. (1947), in *Industrial and Engineering Chemistry,* Vol. 39, p. 517.

Tillerson, J.R., and F.B. Nimick (1984), *Geoengineering Properties of Potential Repository Units at Yucca Mountain, Southern Nevada,* prepared by Sandia National Laboratories for the U.S. Department of Energy, SAND84-0221, December 1984.

Todd, D.K. (1980), *Groundwater Hydrology,* John Wiley and Sons, New York, New York.

Thompson, G.M., J.M. Hayes, and S.N. Davis (1974), *Fluorocarbon Tracers in Hydrology,* Geophysical Research Letters. Vol. 1, No. 4, pp. 177–180.

Van Genuchten, R. (1978), *Calculating the Unsaturated Hydraulic Conductivity With a New Closed Form Analytical Model,* Water Resources Bulletin, Princeton University Press, Princeton University, Princeton, New Jersey.

Verma, A., K. Pruess, C.F. Tsang, and P.A. Witherspoon (1985), "A Study of Two-Phase Concurrent Flow of Steam and Water in an Unconsolidated Medium," in *Proceedings of the 23rd ASME/AIChE National Heat Transfer Conference*, Denver, CO, August 4–7, 1985.

Wang, J.S.Y., and T.N. Narasimhan (1984), *Hydrologic Mechanisms Governing Fluid Flow in Partially Saturated, Fractured, Porous Tuff at Yucca Mountain*, Lawrence Berkeley Laboratory Report, LBL-18473, University of California, Berkeley, California.

Ward, J.S., and N.R. Morrow (1985), "Capillary Pressure and Gas Relative Permeabilities in Low-Permeability Sandstone," in the *Proceedings of the 1985 SPE/DOE Joint Symposium on Low Permeability Reservoirs*, May 19–22, 1985, Denver, Colorado, pp. 321–334.

White, D.E., J.D. Hem, and G.A. Waring (1963), *Data of Geochemistry, 6th Edition*, Ch. F, Geological Survey Professional Paper 440-F, U.S. Government Printing Office, Washington, D.C.

Wilder, D.G., F. Rogue, W.R. Beloff, E. Binnall, and E.C. Gregory (1982), *Executive Committee Report, Geotechnical Instrumentation Working Group Meeting*, at Denver, Colorado, Dec. 2 and 3, 1981, presented at the American Society of Civil Engineers Conference, Geotechnical Conference and Exhibit, Las Vegas, Nevada, April 26–28, 1982, Lawrence Livermore National Laboratory Report UCRL-87183, Livermore, California.

Witherspoon, P.A., N.G.W. Cook, and J.E. Gale (1980), *Progress with Field Investigations at Stripa*, Lawrence Berkeley Laboratory Report LBL-10559, SAC-27. University of California, Berkeley, California.

Wolery, T.J. (1979), *Calculation of Chemical Equilibrium Between Aqueous Solutions and Minerals: The EQ3/EQ6 Software Package*, Lawrence Livermore National Laboratory, Livermore, California, UCRL-52658.

Wollenberg, H.A., H.R. Bowman, and F. Asaro (1977), *Geochemical Studies at Four Northern Nevada Hot Spring Areas*, Lawrence Berkeley Laboratory, Berkeley, California, LBL-6808.

Wollenberg, H.A. and A.R. Smith (1985), *Naturally-Occurring Radioelements and Terrestrial Gamma-Ray Exposure Rates*, Lawrence Berkeley Laboratory, Berkeley, California, LBL-18741.

Wollenberg, H.A., S. Flexser, and L. Andersson (1980), *Petrology and Radiogeology of the Stripa Pluton*, Lawrence Berkeley Laboratory, Berkeley, California, LBL-11654.

Zimmerman, R.M., M.P. Board, E.L. Hardin, and M.D. Voegele (1984), "Ambient Temperature Testing of the G-Tunnel Heated Block," *Proceedings of the 25th Symposium on Rock Mechanics*, Evanston, Illinois, pp. 281–295, June 25–27, 1984.

Zimmerman, R.M. (1982), *Preliminary Design and Definition of Field Experiments for Welded Tuff Rock Mechanics Program*, Sandia National Laboratories Report SAND81-1972, Albuquerque, New Mexico, June 1982.

Zimmerman, R.M., M.L. Wilson, M.P. Board, M.E. Hall, and R.L. Schuch (1985), "Thermal Cycle Testing of the G-Tunnel Heated Block," *Proceedings of the 26th U.S. Symposium on Rock Mechanics*, Vol. 2, Rapid City, SD, pp. 749–758, June 26–28, 1985.

APPENDIX

DIFFUSIVE TRANSPORT OF GASEOUS RADIONUCLIDES

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May 1986

Revised December 1986

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DIFFUSIVE TRANSPORT OF GASEOUS RADIONUCLIDES

Introduction

The migration of various gaseous radionuclides such as iodine-129, carbon-14, and krypton-85 away from repositories is of concern (Roseboom, 1983). These gases along with others are expected to be released from high level waste canisters as they inevitably deteriorate. To date there appears to have been few analyses of rates at which gaseous radionuclides will reach the accessible environment. Much of the work to date on the possible use of the vadose zone for disposal of high level waste has hinged on advantages of a partially saturated matrix. In particular, the vadose zone generally offers an environment with low hydraulic conductivities and high storage capacities. However, the same conditions which decrease rates of liquid phase transport also enhance gaseous transport. Thus there appear to be trade-offs in waste isolation that arise from the competing mechanisms involved in aqueous and gaseous transport. This appendix will provide an outline of mechanisms of gaseous transport, and some suggestions for future investigations. The various modes of gaseous transport of radionuclides through fractured porous media will be considered in the following sections. Only the mechanism of ordinary diffusion will receive detailed review. The other mechanisms of gaseous transport which will be addressed briefly are convection, thermal diffusion, and forced diffusion. The special attention given to the mechanism of ordinary diffusion does not imply that these other mechanisms are expected to contribute less significantly to total gaseous fluxes from repositories.

A review of some methods for experimentally measuring porous media gas diffusivities will be presented following the sections on the various mechanisms for gaseous transport. A possible approach to making field scale measurements of gas diffusion in tuff is also considered.

Other recent reviews addressing transport of radionuclides from a high-level waste repository in unsaturated porous rock include the works of Rasmussen and Evans (1986), and Green and Evans (1987).

Convection

Convective transport of gases occurs in response to a gradient in total gas pressure. In porous media, isothermal convective transport is described by Darcy's law for compressible fluids (Scheidegger, 1974). In the absence of gradients of temperature and gas composition, the molar flux density of the i^{th} gas species through an isotropic porous medium is

$$\vec{N}_i = -X_i P_o \frac{k_g}{RT\mu}(\nabla P_o - \rho_o \vec{g}) \text{ ,} \qquad \text{(A.1)}$$

where X_i is the mole fraction of the i^{th} species, P_o is the total gas pressure, k_g is the gas permeability, R is the gas constant, T is the Kelvin temperature, μ is the dynamic viscosity, ρ_o is the gas density, and $\vec{g}$ (in the direction of -z) is the acceleration due to gravity. k_g is more generally a tensor quantity (or much worse in heterogeneous media), and is also strongly dependent on the volumetric gas content (or conversely, on the volumetric water content). Furthermore, over a finite volume, the gas density will generally vary due to high compressibility of the gas.

The preceding discussion is generally valid for isothermal convection at low Reynold's numbers, N_{Re}, and at low Knudsen numbers, N_{Kn}. This latter condition is of special interest. N_{Kn} is defined as the ratio of the gas mean free path, l_o, to the characteristic pore radius, r_o. When larger N_{Kn} are attained, "slip flow" becomes significant. In slip flow, the observed flux is greater than that predicted by the product of ∇P and the conventionally used k_g. The analysis of slip flow is generally associated in the earth sciences literature with the work of Klinkenberg (1941). This work, as well as other works on slip flow, are reviewed by Scheidegger (1974). Klinkenberg accounted for the slip phenomenon by expressing k_g as a function of the average gas pressure $\bar{P}_o$, the gas permeability at high pressures k_∞, and a further empirical constant b. In Klinkenberg's equation

$$k_g = k_\infty\left[1 + \left(\frac{b}{\bar{P}_o}\right)\right] \text{ ,} \qquad \text{(A.2)}$$

it is implicit that k_∞ and b are not only specific to a given porous medium but also to a specific water content and gas composition.

Slip flow is more pronounced in less permeable media, becoming observable in the millidarcy range. Reported values of saturated matrix hydraulic conductivities (Peters *et al.*, 1984) indicate that most matrix permeabilities for Yucca Mountain tuff are well below the millidarcy range. Reda (1985) measured gas permeabilities on densely welded Paintbrush Tuff, and observed slip flow in the microdarcy range.

Within the various tuff formations at Yucca Mountain, convective gas transport could occur through both desaturated matrix pores and desaturated fractures. While the fracture porosity is much lower than that of the matrix (*e.g.*, Sinnock *et al.*, 1984), transport through fractures is likely to have disproportionately greater influence for at least three reasons. First, aside from slip-flow effects, velocity profiles across pore and fracture spaces tend to be parabolic (as in Poiseuille flow). Such velocity profiles greatly enhance convection through the generally larger fractures. Secondly, due to the large proportion of very fine pores, much of the matrix may be expected to remain water-saturated. Thus, the full matrix porosity is not likely to contribute to gas flow. Thirdly, there is some evidence that not all matrix pores are interconnected (Peters *et al.*, 1984). All of these factors lead to the expectation that fracture gas permeabilities are always much larger than matrix gas permeabilities. Field-scale air permeability measurements would be required to properly determine k_g. Works addressing such methods include those of Stallman (1967) and Weeks (1977), although applicability at a scale appropriate for characterizing the Yucca Mountain site is uncertain.

The magnitude of gas pressure gradients associated with various possible repository conditions needs to be determined. An initial local P_o increase is expected upon canister emplacement as a consequence of increased local temperatures. This effect is due not only to the response of gas expansion, but also to vaporization of local matrix pore waters. The significance of this initial P_o requires further analysis. After the temperature profile has stabilized and ∇P_o has dissipated, convective transport could continue due to lower gas phase densities around the repository. Counter-flows of water towards heat sources and vapor away from heat sources have been analyzed in various heat pipe studies (*e.g.*, Luikov, 1975; Udell, 1983; Pruess, 1985; and Pruess *et al.*, 1985). Further disturbances could also introduce subsequent pressure gradient driven convection. These later events could include emplacement of more canisters and failure of existing canisters.

Convective transport resulting from disturbances at the soil surface has been reviewed in a number of works in soil physics (*e.g.*, Baver *et al.*, 1972; Marshall and Holmes, 1979). Soil surface gradients in P_o arise from barometric pressure fluctuations, surface thermal gradients, soil water content changes, and wind eddies. These surface causes of convective gas transport are generally regarded as minor in comparison to diffusive transport. However, a study by Clements and Wilkening (1974) on radon fluxes out of soil, correlated atmospheric pressure changes with changes in radon flux as large as 60%. This suggests that convective gas flow from barometric pressure fluctuations can become comparable to diffusive transport.

Thermal Diffusion

In the presence of a temperature gradient, there exists a weak tendency for net flow of individual gas species in a mixture, even in the absence of other driving forces such as gradients in total or partial pressures. This process which is solely driven by temperature gradients is referred to as thermal diffusion (Kennard, 1938). Thermal diffusion in gases was theoretically predicted by Chapman in 1916, and later experimentally verified.

Thermal diffusion is generally a small effect. This is especially true for mixtures of gases with comparable masses, and for softer intermolecular repulsion forces. The relative importance of thermal diffusion to that of ordinary diffusion is often expressed through a factor k_T, the thermal diffusion ratio. k_T is defined as the ratio of the thermally induced flux to that due to a composition gradient when $\frac{1}{T}\frac{\partial T}{\partial x}$ and $\frac{1}{n_o}\frac{\partial n_i}{\partial x}$ are equal. Here n_o and n_i are the total molecular number density and number density of the i^{th} species, respectively. For hard-sphere

86

repulsion of similar gases, $k_T < 0.01$. For hard-sphere repulsion of gases of very different masses such as Ar and He, or O_2 and H_2, $k_T \approx 0.13$. The usual tendency in thermal diffusion is for the heavier molecular species to drift toward regions of lower temperature. This tendency would enhance transport of the heavier volatile radionuclides away from the repository.

Estimates of the expected temperature distributions at the repository in both time and space are needed to predict the influence of thermal diffusion. The studies by Klasi *et al.* (1982a,b) provide simulated temperature profiles for various scenarios for a repository at 800 m in tuff. The analyses included thermal loadings ranging from 25 to 150 kW/acre, and also considered cases with and without boiling of pore waters. Temperature profiles from analyses such as these could be used to estimate the possible significance of thermal diffusion. Laboratory and field heater experiments provide the most direct measure of various transport processes under thermal gradients. Examples of heater experiments include those of Eaton *et al.* (1983) and Johnstone *et al.* (1984).

Forced Diffusion

In the presence of external force fields, transport can occur even in the absence of gradients in temperature, total pressure, or partial pressures. Forced diffusion is generally associated with net drift of ionic species in the presence of an electric field. While usually considered an insignificant effect in gas diffusion through porous media, the environment created by a nuclear waste repository provides conditions conducive to forced diffusion. The electric field would be induced by Compton scattered electrons generated by gamma radiation from the decay of high level waste. Green *et al.* (1985) have analyzed two extreme pathways for forced diffusion away from a repository. These cases are that of forced diffusion through a rock mass, and forced diffusion through open air. The latter case is associated with transport through large fractures and open boreholes. Their study concluded that forced diffusion appears potentially significant only in the case of open air channels. They recommend further study directed at the more realistic cases of systems with intermediate transport capabilities.

Ordinary Diffusion (Continuum, Transition, and Knudsen)

Transport of various gaseous species driven solely by gradients in partial pressure is referred to as ordinary diffusion. Continuum, transition, and Knudsen diffusion can be regarded as extensions of ordinary gaseous diffusion resulting from varying degrees of importance of gas molecule collisions with a solid (or more generally the condensed phase) matrix. As noted earlier, the Knudsen number N_{Kn} is defined as the ratio of the mean free path between intermolecular collisions (in a simple gas phase) l_o, to a characteristic pore dimension r_o. Continuum diffusion adequately describes partial pressure gradient driven transport in the limit of $N_{Kn} << 1$. In this limit, gas molecules collide primarily with other gas molecules. In the opposite limit of large Knudsen numbers ($N_{Kn} >> 1$), Knudsen diffusion describes transport in which gas molecules collide almost exclusively with pore walls. Transition range diffusion refers to diffusion in intermediate ranges of N_{Kn}. While the field environment is one where numerous gas species interdiffuse simultaneously, the following discussion will be restricted to simple cases of self-diffusion and binary gas diffusion. Consideration of simple cases will still address the relevant processes found in the more complex field situation.

The vast majority of studies on gas diffusion in porous media express the effective porous media diffusivity of species i in species j, D_e^{ij}, as some linear function of the ordinary diffusivity of species i and j in a simple gaseous system, D_o^{ij}. It is instructive to consider the nature of D_o^{ij} first, before addressing the effect of the porous medium on diffusion. A qualitative appreciation of ordinary diffusion can be gained through the simple kinetic theory of self-diffusion. This approach results in expressing the self-diffusion coefficient as

$$D_o^{ii} = \frac{1}{3} \bar{v} l_o \ , \qquad \text{(A.3)}$$

where $\bar{v}$ is the mean speed of the molecules, and l_o is the mean free path between intermolecular collisions. The mean speed is to a good approximation equal to the Maxwell mean speed which is solely determined by the molecular mass m_i, and the Kelvin temperature T.

$$\bar{v} = \left[\frac{8k_B T}{\pi m_i} \right]^{1/2} , \qquad \text{(A.4)}$$

where k_B is the Boltzmann constant. The mean free path is given approximately by

$$l_o = \frac{1}{\sqrt{2}\pi\sigma^2 n_o} , \qquad \text{(A.5)}$$

where σ is the diameter of the molecules and n_o is their number density. Using the ideal gas law with Eq. (A.5) gives

$$l_o = \frac{k_B T}{\sqrt{2}\pi\sigma^2 P_o} , \qquad \text{(A.6)}$$

where P_o is the total pressure. Substituting equations (A.4) and (A.6) into equation (A.3) demonstrates the mass, pressure, and temperature dependencies of gas diffusivities. Diffusion is mass dependent through $\bar{v}$ as $m^{1/2}$. The pressure dependence enters through l_o as P_o^{-1}. The data on the temperature dependence of diffusivities does not however appear as $T^{3/2}$ as may be inferred from simple kinetic theory. Instead of (3/2), the exponent tends to range from about 1.7 to 2.0, depending on the gas species. This discrepancy is qualitatively attributed to a temperature dependence of the collision cross-section (assumed constant in the hard-sphere simple kinetic theory). The above considerations serve to emphasize the strong temperature dependence and inverse pressure dependence of ordinary gas diffusion.

Nearly all studies on porous media gas diffusion in the earth sciences literature express D_e^{ij} as a scalar reduction of D_o^{ij}. Much of the work addressing D_e in the chemical engineering literature also conforms to this approach. The reducing factor, $f(\phi_g)$, serves to decrease D_o^{ij} through the gas phase porosity ϕ_g, and through a tortuosity factor τ. Thus (dropping the understood superscripts),

$$D_e = f(\phi_g)D_o \qquad \text{(A.7)}$$

A number of proposed forms for $f(\phi_g)$ are reviewed in Youngquist (1970), van Brakel and Heertjes (1974), Troeh *et al.* (1982), and Mitani (1984). These and other proposed expressions for $f(\phi_g)$ are listed in Table A.1. Implicit in the use of D_e in forms fitting equation (A.7) is the condition that $N_{Kn} << 1$. In this limit, the gas phase behaves as a continuum. Among the many works cited in these and other papers, there is nearly universal agreement that f is linear in ϕ_g to the extent that this parameter is equal to the volume-averaged available gas phase area per unit bulk area. A number of works define τ as the ratio of the macroscopic path length L to the longer (tortuous) diffusion path length L_e. This approach generally leads to the intermediate result of

$$D_e = \phi_g \tau^2 D_o \ . \qquad \text{(A.8)}$$

Some studies define τ as the inverse of the definition used here. In any case, tortuosity is a vague concept. Due to the ambiguity of the factor τ (recognized at least as early as Carman, 1956), the majority of workers have attempted to express τ as a function of ϕ_g. This results in a variety of nonlinear dependencies of D_e on ϕ_g, many of which are mentioned in the previously cited works. van Brakel and Heertjes demonstrate that there is no general theoretical basis for expressing τ as a function of ϕ_g. They further argue that a third parameter is needed along with ϕ_g and τ to determine D_e. That third parameter is a constrictivity, δ, used to account for variations in accessible cross-sectional areas along diffusion paths.

Most models for gas diffusion in porous media implicitly or explicitly regard the presence of any liquid phase as being equivalent to an impervious solid phase. In these models the volumetric liquid content (liquid volume per unit bulk volume) ϕ_l acts only to reduce the portion of the total porosity (ϕ_o) available to the gas phase. This approach is usually justified since diffusivities of most species in liquids are of the order of 10^{-4} that of their respective gas phase diffusivities. Ignoring dissolved gas diffusion through liquid saturated pores does result in significant modelling errors in cases where ϕ_l approaches ϕ_o. This may be the condition of much of the tuff matrix at Yucca Mountain (*e.g.*, Sinnock *et al.*, 1984, Table 3). Nielson *et al.* (1984) have developed a model for diffusion through both air-filled and water-filled pores. Sallam *et al.* (1984) reported measurements of D_e in soil at low ϕ_g, and compared their results with two models for predicting D_e. They found that Penman's (1940) model greatly overestimated D_e, while that of Millington and Quirk (1961) slightly underestimated D_e.

In the limit of large N_{Kn}, equations of the form of (A.7) and (A.8) greatly overestimate D_e.

Table A.1. Some Proposed Forms of $f(\phi_g)$*

$f(\phi_g)$	Source	Notes
ϕ_g^2	Buckingham (1904)	...
$\dfrac{\phi_g}{1+(k-1)(1+\phi_g)}$	Burger (1919)	k is a shape factor
$\dfrac{2}{3}\phi_g$	Penman (1940)	...
$0.668\phi_g$	Taylor (1949)	...
$0.58\phi_g$	van Bavel (1952)	...
$\phi_g^{3/2}$	Marshall (1959)	...
$\phi_g^{4/3}$	Millington (1959)	...
$\gamma\phi_g^{\mu}$	Currie (1960)	$0.8 \leqslant \gamma \leqslant 1$, $\mu \leqslant log(f)/log\phi_g$
$\phi_g^{3.33}\phi_o^{-2}$	Millington & Quirk (1961)	...
$\leqslant \dfrac{\phi_g}{1+0.5(1-\phi_g)}$	Hashkin & Shtrickman (1962)	...
$\leqslant \dfrac{\phi_g}{1-0.5ln\,\phi_g}$	Weissberg (1963)	overlapping spheres
$\phi_g^{5/3}$	Shearer et al. (1966)	...
$\left[\dfrac{\phi_g-u}{1-u}\right]^v$	Troeh et al.(1982)	$0 \leqslant u \leqslant \phi_g$, $1 \leqslant v \leqslant 2$
$\phi_g^{3.10}\phi_o^{-2}$	Sallam et al. (1984)	$\phi_g \leqslant 0.15$

*The effects of tortuosity, τ, are expressed through ϕ_g.

Due to the increased importance of gas molecule collisions with pore walls in this limit, trajectory lengths become more dependent on pore dimensions rather than the proximity of other gas molecules. In the Knudsen limit,

$$D_e = \frac{1}{3} f\left(\phi_g\right) \bar{v}r_o \ . \qquad \text{(A.9)}$$

At 298° K and 1 atm, $l_o \approx 10^{-7}$m for O_2 and N_2. At the same pressure, but at twice that temperature, l_o would only be about doubled. Thus the Knudsen limit ($l_o >> r_o$) could only be realized in extremely fine pores. Therefore, the desaturated portions of a tuff matrix could be expected to exhibit both slip flow and transition regime diffusion. It is conceivable that Knudsen diffusion would take place in the immediate vicinity of a repository; however, at distances far enough removed to allow water condensation it appears likely that the finer pores would be water saturated.

While Knudsen limit diffusion appears to be an exceptional case, diffusion in the transition range between the Knudsen and continuum limits seems more generally possible. Conditions where $N_{Kn} \approx 1$ are likely within the rock matrix. A treatment of the transition range for gas diffusion was developed by Bosanquet in 1944 (cited in Pollard and Present, 1948). This expression

89

$$D_e^{-1} = \left[f(\phi_g) D_o \right]^{-1} + D_{Kn}^{-1} \quad , \quad \text{(A.10)}$$

where D_{Kn} is the Knudsen diffusivity (identical to equation A.9), has been derived from a variety of approaches (*e.g.*, Pollard and Present, 1948; Evans *et al.*, 1961; Spiegler, 1966; Ho and Strieder, 1980; and Tokunaga, 1985). Equation A.10 has further utility in being applicable even in the Knudsen and continuum limits. The Bosanquet equation has been incorporated in the previously mentioned work of Nielson *et al.* (1984).

The variety of expressions for D_e, along with the numerous restrictions placed on many models (*e.g.*, isotropic media, or specific pore geometries) suggest that experimentally determined D_e will be required in studying diffusion in complex natural systems. The diversity of theoretical models are however useful in indicating the expected magnitude of D_e.

Methods for Measuring Gas Diffusion in Fractured Porous Media

This section provides a survey of laboratory and field methods for measuring gas diffusion through fractured porous media. The existing methods reviewed here are primarily from the soil science and chemical engineering literature. While these methods have not been developed for the purpose of testing fractured porous media, much of the technology appears transferable. These methods are generally suited for measuring rock matrix D_e, although shorter sample lengths and longer diffusion times may be required due to the expected low values of D_e. For measuring laboratory samples which include fractures, additional steps for data interpretation will be required due to expected high contrasts in matrix and fracture diffusivities. Contrasts in diffusivities arise from two features of fractured porous media. First, the fracture tortuosity effects tend to be of less importance than in the matrix (along the general direction of a fracture surface or channel). Second, due to the generally smaller dimensions of matrix pores, wall collisions in the matrix tend to result in lower D_e. Both of these effects result in larger D_e within fractures (along directions of fracture planes). When measuring diffusion in the direction of a fracture plane, lateral diffusion from the fracture into the rock matrix must be accounted for. An excellent review of methods for measuring gas diffusion is provided by Marrero and Mason (1972). Their work is directed at measurement of D_o^{ij} rather than D_e^{ij}, yet many useful comments are provided regarding limitations of various methods. That study also includes a very comprehensive list of D_o^{ij} measurements. For field measurements, none of the existing methods appears directly suited for obtaining the required large-scale, volume-averaged D_e. One possible method for measuring D_e on the field scale is presented at the close of this section.

Laboratory methods for measuring gas diffusion coefficients in porous media may be categorized into steady-state and transient methods. Examples of steady-state methods include those by Buckingham (1904), Penman (1940), Wicke and Kallenbach (1941), van Bavel (1952, in which a correction to Penman's method is also noted), and Weisz (1957). The methods of Penman and van Bavel utilize evaporation from a volatile liquid to establish one constant partial pressure boundary, while venting the opposite boundary to the atmosphere so that steady state diffusion becomes established. The methods of Buckingham, Wick and Kallenbach, and Weisz induce steady-state counterdiffusion by imposing steady streams of gases (of equal total pressure, and differing composition) at opposite ends of the porous medium. As noted by Hoogschagen (1953) and Evans *et al.* (1961), the ratio of the counterdiffusing fluxes is equal to the inverse square-root of the molecular weight ratios, rather than being equal to unity as assumed by many other analyses (*e.g.*, Buckingham, 1904; Wicke and Kallenbach, 1941; Wheeler, 1951; and Weisz and Prater, 1954).

There also exists a class of indirect steady-state methods for estimating D_e. In these approaches, some other transport property analogous to gas diffusion is measured in both the porous medium and a single phase (usually a liquid). For porous media of negligible electrical conductivity, the electrical conductivity of an electrolyte-saturated sample can be measured and compared with that of the electrolyte solution alone. The ratio of the former to the latter can then be equated with $f(\phi_g)$. This technique has been employed by Klinkenberg (1951), and Scott and Dullien (1962). The work on solute diffusion in tuff by Walter (1982) may also be interpreted from this perspective as providing information on $f(\phi_g)$ for gases in completely desaturated media. In light of Knudsen effects, however, indirect approaches to D_e are not generally reliable.

One dimensional, transient methods can be divided into open-tube and closed-tube methods. In open-tube methods, one end of the sample is open to either atmospheric air or some other extremely large volume of gas, effectively establishing a constant concentration boundary condition. The methods of Taylor (1949), Currie (1960), Papendick and Runkles (1965), and Bakker and Hidding (1970) are of this category. A generalization of the open-tube approach in which time dependent boundary gas concentrations are used is given by Rolston and Brown (1977).

Closed-tube methods have several advantages over open-tube methods. In closed systems, hazardous or expensive gases can be contained and conserved. Closed-tube methods can allow for experiments at total pressures other than atmospheric. Finally, a closed system can be placed in a temperature regulation bath for greater temperature control. Closed-tube methods can be further subdivided into dual and single end chamber methods. Dual end chamber methods consist of a sample column with opposite ends exposed to gas chambers. The dissipation of initial gas concentration differences (in the absence of total pressure differences) can be monitored at either or both end chambers. The methods of Dye and Dallavalle (1958), Ball *et al.* (1981), Reible and Shair (1982), and Sallam *et al.* (1984) are dual chamber methods. In single end chamber, closed-tube methods only one end of the sample column is exposed to an end chamber in which gas composition is monitored. Rust *et al.* (1957) have presented a single end chamber method.

The following methods for determining D_e in the field are all from the soil science literature. McIntyre and Philip (1964) designed a diffusion chamber consisting of a tube inserted into the soil surface and a well-stirred end chamber in which gas composition is monitored. The gas composition in the end chamber is initially set unequal to that within the soil. The transient, one-dimensional diffusion between the soil in the tube and the end chamber is monitored to obtain D_e. Lai *et al.* (1976) developed a transient radial diffusion method. In their work, oxygen gas was injected with a syringe into soil at a particular depth. The time dependent concentration of oxygen at the injection point was periodically monitored by withdrawing small sample gas volumes from the injection point, and D_e was obtained from an analytic solution to the radial diffusion problem. The previously mentioned work of Rolston and Brown (1977) was also used to measure D_e in the field. In the reported application, a soil surface area of 0.25 m^2 was covered with a box in which argon gas was pumped.

A common apparent limitation of the above methods is that of the limited volume over which D_e is measured. Extension of the methods of McIntyre and Philip, and of Rolston and Brown to areas of the order of 100 m^2 or larger seem cumbersome. On the other hand, the method of Lai *et al.* may, with some modifications, prove useful in field scale D_e measurements at Yucca Mountain.

A large underground chamber such as a sealed mine shaft or an otherwise isolated section of a tunnel may be equipped to serve as a "well-stirred" volume in which gas composition and pressure could be remotely monitored in a transient diffusion experiment. An initially high concentration of the gas to be monitored could be released in the chamber at time zero, and its dissipation monitored with time. If the surrounding rock behaves sufficiently like a homogeneous, isotropic porous medium, the method of Lai *et al.* could be applied directly. More realistically, the surrounding rock may be characterized as a heterogeneous, anisotropic, fractured porous medium. Even in this more complex case, experimental data could still be numerically inverted to provide estimates of D_e. To better characterize heterogeneities, neighboring boreholes could be packed off and used as monitoring points as well as additional sources (using different tracer gases). An experiment of this type is expected to require time of the order of about one year of periodic monitoring, to characterize regions within around 10 m from each source cavity. Due to the extremely large volume of rock requiring characterization, the gas species to be monitored should ideally be detectable at very low concentrations, adsorb very weakly on mineral surfaces, and have very low solubility in water. A gas satisfying these criteria is freon, CCl_2F_2 (*e.g.*, Sallam *et al.*, 1984). Field experiments following these rough guidelines should provide much needed information on diffusive gas transport, with relatively simple techniques, and at low costs. With further modifications in this experimental design, field tests of gas transport under various combinations of driving forces (gradients in partial pressure, total pressure, and temperature) seem equally feasible.

Concluding Remarks

A variety of mechanisms for gaseous transport and diffusion measurement methods have been briefly considered. While the actual field problem will be one of multiple species transport in response to coupled driving forces, this simple discussion provides an introduction to several of the basic processes involved. The importance of field testing for gaseous transport can not be emphasized enough. Such work will fill a large gap in site characterization. The effects of individual as well as coupled processes could be measured at the appropriate scale. The impact of several complex processes may not be assessed confidently solely from theoretical methods. The field problem will include not only the previously mentioned mechanisms but others such as aerosol transport, adsorption-desorption, liquid phase transport, chemical reactions, and radioactive decay. A set of well designed field tests could assess the impact of these simultaneous processes. While the relative effects of individual mechanisms will probably not be well understood, the composite result of simultaneous transport processes is of ultimate concern.

REFERENCES

Bakker, J.W., and A.P. Hidding, 1970. The influence of soil structure and air content on gas diffusion in soils. *Netherlands J. Agric. Sci., 18:* 37–48.

Ball, B.C., W. Harris and J.R. Burford, 1981. A laboratory method to measure gas diffusion and flow in soil and other porous materials. *J. Soil Sci. 32:* 323–333.

Baver, L.D., W.H. Gardner and W.R. Gardner, 1972. *Soil Physics.* 4th edition, John Wiley and Sons, Inc., New York.

Buckingham, Edgar, 1904. Contributions to our knowledge of the aeration of soils. *U.S.D.A. Bureau of Soils, Bull. #25.*

Burger, H.C., 1919. Das Leitvermogen verdunnter mischkristallfreier Legierungen. *Physik Zs., 20:* 73–75.

Carman, P.C., 1956. *Flow of Gases through Porous Media.* Butterworths Scientific Publication, London.

Clements, William E., and Marvin H. Wilkening, 1974. Atmospheric pressure effects on ^{222}Rn transport across the earth-air interface. *J. Geophys. Research, 79* (33), 5025–5029.

Currie, J.A., 1960. Gaseous diffusion in porous media. Part 1. A non-steady state method. *British J. Appl. Phys. 11:* 314–317.

Dye, R.F., and J.M. Dallavalle, 1958. Diffusion of gases in porous media. *Ind. Eng. Chem., 50* (8), 1195–1200.

Eaton, Roger R., J. Keith Johnstone, Jace W. Nunziato and Chris M. Korbin, 1983. *In-situ tuff water migration/heater experiment. Post-test thermal analysis.* Sandia Report, SAND 81-0912, October.

Evans, R.B., G.M. Mason and E.A. Mason, 1961. Gaseous diffusion in porous media at uniform pressure. *J. Chem. Phys. 35* (6) 2076–2083.

Green, Ronald T., and Daniel D. Evans, (expected 1987). *Radionuclide transport as vapor through unsaturated rock.* Prepared for the U.S. Nuclear Regulatory Commission, October 1986, NUREG/CR-4654.

Green, R.T., W. Filippone and D.D. Evans, 1985. Radionuclide transport as vapor in a non-isothermal dual porosity system. *Proceedings International Symposium on Coupled Processes Affecting the Performance of a Nuclear Waste Repository.* Lawrence Berkeley Laboratory, September 18–20, pp. 155–160.

Hashkin, A., and S. Shtrikman, 1962. A variational approach to the theory of the effective magnetic permeability of multiphase materials. *J. Appl. Phys. 33:* 3125.

Ho, Fun Gan, and William Strieder, 1980. Numerical evaluation of the porous medium effective diffusivity between the Knudsen and continuum limits. *J. Chem. Phys. 73* (12): 6296–6300.

Hoogschagen, J., 1953. Equal pressure diffusion in porous substances. *J. Chem. Phys., 21:* 2096–2097.

Johnstone, J. Keith, G. Ronald Hadley, and David R. Waymire, 1984. *In-situ tuff water migration/heater experiment. Final Report,* Sandia National Laboratories, SAND 81-1918, June 1984.

93

Kennard, Earle H., 1938. *Kinetic Theory of Gases* (with an introduction to statistical mechanics). McGraw-Hill Book Co., Inc., New York.

Klasi, Melvin L., William C. McClain and Terje Brandshaug, 1982a. *Far-field thermal analysis of a spent fuel repository in tuff.* SAND 81-7209, Sandia National Laboratories, Albuquerque, New Mexico.

Klasi, Melvin L., James E. Russell, William C. McClain, and Terje Brandshaug, 1982b. *Far-field thermal analysis of a high level waste repository in tuff.* SAND 81-7210, Sandia National Laboratories, Albuquerque, New Mexico.

Klinkenberg, L.J., 1941. The permeability of porous media to liquids and gases. American Petroleum Institute (API), *Drilling Production Practice,* 200–213.

Klinkenberg, L.J., 1951. Analogy between diffusion and electrical conductivity in porous rocks. *Bull. Geol. Soc. America, 62:* 559–564.

Lai, Sung-Ho, James M. Tiedje and A. Earl Erickson, 1976. In situ measurement of gas diffusion coefficient in soils. *Soil Sci. Soc. Amer. J., 40:* 3–6.

Luikov, A.V., 1975. Systems of differential equations of heat and mass transfer in capillary-porous bodies (review), *Int. J. Heat Mass Transfer, 18:* 1–14.

Marrero, T.R., and E.A. Mason, 1972. Gaseous diffusion coefficients. *J. Chem. Phys. Ref. Data., 1:* 3–118.

Marshall, T.J., 1959. The diffusion of gases through porous media. *J. Soil Sci., 10* (1): 79–82.

Marshall, T.J., and J.W. Holmes, 1979. *Soil Physics.* Cambridge University Press.

McIntyre, D.S., and J.R. Philip, 1964. A field method for measurement of gas diffusion into soils. *Aust. J. Soil Res., 2:* 133–145.

Millington, R.J., 1959. Gas diffusion in porous media. *Science, 130:* 100–102.

Millington, R.J., and J.P. Quirk, 1961. Permeability of porous solids. *Trans. Faraday Soc., 57:* 1200–1207.

Millington, R.J., and R.C. Shearer, 1971. Diffusion in aggregated porous media. *Soil Sci., 111* (6): 372–378.

Mitani, Masashi, 1984. Geometric factor for diffusion in porous media. *J. of Chem. Engineering Japan, 17* (4): 441–443.

Nielsen, K.K., V.C. Rogers and G.W. Gee, 1984. Diffusion of radon through soils: A pore distribution model. *Soil Sci. Soc. America J., 48* (3): 482–487.

Pappendick, R.L., and J.R. Runkles, 1965. Transient state oxygen diffusion in soil. *Soil Sci. 100:* 251–261.

Penman, H.L., 1940. Gas and vapour movements in the soil: I. The diffusion of vapours through porous solids. *J. Agric. Sci., 30:* 437–462.

Peters, R.R., E.A. Klavetter, I.J. Hall, S.C. Blair, P.R. Heller and G.W. Gee, 1984. *Fracture and matrix hydrologic characteristics of tuffaceous materials from Yucca Mountain, Nye County, Nevada.* SAND 84-1471, Sandia National Laboratories, Albuquerque, New Mexico.

94

Pollard, W.G., and R.D. Present, 1948. On gaseous self-diffusion in long capillary tubes. *Physical Review, 73* (7): 762–774.

Pruess, Karsten, 1985. *TOUGH User's Guide.* Lawrence Berkeley Laboratory, LBL 20700, November.

Pruess, K., J.S.Y. Wang and Y.W. Tsang, 1985. *Effective continuum approximation for modeling fluid and heat flow in fractured porous tuff.* Lawrence Berkeley Laboratory, LBL 20778.

Rasmussen, Todd C., and Daniel D. Evans, 1986. *Unsaturated flow and transport through fractured rock — Related to high-level waste repositories — Phase II.* Prepared for the U.S. Nuclear Regulatory Commission, NUREG/CR-4655.

Reda, Daniel C., 1985. Slip-flow experiments in welded tuff: The Knudsen diffusion problem. *Proceedings International Symposium on Coupled Processes Affecting the Performance of a Nuclear Waste Repository.* Lawrence Berkeley Laboratory, September 18–20, pp. 191–196.

Reible, D.D., and F.H. Shair, 1982. A technique for measuring gaseous diffusion porous media. *J. Soil Sci., 33:* 165–174.

Rolston, D.E., and B.D. Brown, 1977. Measurement of soil gas diffusion coefficients for a transient-state method with a time-dependent surface condition. *Soil Sci. Soc. Am. J., 41:* 499–505.

Roseboom, Eugene H., Jr., 1983. *Disposal of high-level nuclear waste above the water table in arid regions.* U.S.G.S. Circular #903.

Rust, R.H., A. Klute and J.E. Gieseking, 1957. Diffusion-porosity measurements using a non-steady state system. *Soil Sci., 84:* 453–463.

Sallam, A., W.A. Jury and J. Letey, 1984. Measurement of gas diffusion coefficient under relatively low air-filled porosity. *Soil Sci. Am. J., 48:* 3–6.

Scheidegger, Adrian E., 1974. *The Physics of Flow through Porous Media,* 3rd edition. University of Toronto Press.

Scott, D.S., and F.A.L. Dullien, 1962. Diffusion of ideal gases in capillaries and porous solids. *A.I.Ch.E.J., 8* (1): 113–117.

Shearer, R.C., Millington, R.J., and J.P. Quirk, 1966. Oxygen diffusion through sands in relation to capillary hysteresis: 2. Quasi-steady-state diffusion of oxygen through partly saturated sands. *Soil Sci., 101* (6): 432–436.

Sinnock, Scott, Y.T. Lin and Joseph P. Brannen, 1984. *Preliminary bounds on the expected postclosure performance of the Yucca Mountain repository site, Southern Nevada.* SAND 84-1492, Sandia National Laboratories, Albuquerque, New Mexico.

Spiegler, K.S., 1966. Diffusion of gases across porous media. *Ind. Eng. Chem. Fundamentals, 5:* 529–532.

Stallman, R.W., 1967. Flow in the zone of aeration. *Advances in Hydroscience, 4,* Van Te Chow, ed.

Taylor, S.A., 1949. Oxygen diffusion in porous media as a measure of soil aeration. *Soil Sci. Am. Proc. 14:* 55–61.

Tokunaga, T.K., 1985. Porous media gas diffusivity from a free path distribution model. *J. Chem. Phys., 82* (11): 5298–5299.

Troeh, F.R., J.D. Jabro, and Don Kirkham, 1982. Gas diffusion equations for porous materials. *Geoderma. 27:* 239–253.

Udell, K.S., 1983. Heat transfer in porous media heated from above with evaporation, condensation and capillary effects. *J. Heat Transfer, 105:* 485–492.

van Bavel, C.H.M., 1952. Gaseous diffusion in porous media. *Soil Sci., 73:* 91–104.

van Brakel, J., and P. M. Heertjes, 1974. Analysis of diffusion in macroporous media in terms of a porosity, a tortuosity and a constrictivity factor. *Int. J. Heat Mass Transfer, 17:* 1093–1103.

Walter, G.R., 1982. *Theoretical and experimental determination of matrix diffusion and related solute transport properties of fractured tuffs from the Nevada Test Site.* LA-9471-MS, Los Alamos National Laboratory, Los Alamos, New Mexico.

Weeks, E.P., 1977. *Field determination of vertical permeability to air in the unsaturated zone.* U.S. Department of Interior, Geological Survey, Open-File Report 77-346.

Weissberg, Harold L., 1963. Effective diffusion coefficient in porous media. *J. Applied Phys., 34* (9): 2636–2639.

Weisz, P. B., 1957. Diffusivity of porous particles. I. Measurements and significance for internal reaction velocities. *Zeitschrift fur Physik. Chem., 11:* 1–15.

Weisz, P. B., and C. D. Prater, 1954. Interpretation of measurements in experimental catalysis. *Adv. Catalysis, 6:* 143–196.

Wheeler, Ahlborn, 1951. Reaction rates and selectivity in catalyst pores. *Adv. Catalysis. 3:* 250–327.

Wicke, Van E., and R. Kallenback, 1941. Die Oberflachendiffusion von Kohlendioxyd in aktiven Kohlen. *Kolloid Zeitschrift, 97:* 135–151.

Youngquist, Gordon R., 1970. Diffusion and flow of gases in porous solids. *Flow through Porous Media,* R.J. Nurge, Chairman, American Chem. Soc. Publications, Washington, D.C., pp. 58–69.

NRC FORM 335
(2-84)
NRCM 1102,
3201, 3202

U.S. NUCLEAR REGULATORY COMMISSION

BIBLIOGRAPHIC DATA SHEET

SEE INSTRUCTIONS ON THE REVERSE

1. REPORT NUMBER *(Assigned by TIDC, add Vol. No., if any)*
NUREG/CR-4161
UCID-20092
Vol. 2

2. TITLE AND SUBTITLE
Critical Parameters for a High-Level Waste Repository, Volume 2: Tuff

3. LEAVE BLANK

4. DATE REPORT COMPLETED

MONTH	YEAR
April	1987

5. AUTHOR(S)
E.P. Binnall, S.M. Benson, L. Tsao, H.A. Wollenberg,
T.K. Tokunaga/Lawrence Berkeley Laboratory
E.M. Didwall/LLNL

6. DATE REPORT ISSUED

MONTH	YEAR
May	1987

7. PERFORMING ORGANIZATION NAME AND MAILING ADDRESS *(Include Zip Code)*
Lawrence Livermore National Laboratory
Post Office Box 808
Livermore, California 94550

8. PROJECT/TASK/WORK UNIT NUMBER

9. FIN OR GRANT NUMBER
A0367

10. SPONSORING ORGANIZATION NAME AND MAILING ADDRESS *(Include Zip Code)*
Division of Engineering
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Washington, DC 20555

11a. TYPE OF REPORT
Technical

b. PERIOD COVERED *(Inclusive dates)*

12 SUPPLEMENTARY NOTES

13 ABSTRACT *(200 words or less)*

This report addresses critical parameters specific to a repository in tuff, using the Yucca Mountain tuffs of Nevada as the principal example. For the purposes of this report, a parameter is considered to be a physical property whose value helps determine the characteristics or behavior of a repository system. Parameters which are defined as critical are those essential to evaluate and/or monitor leakage of radionuclides from the repository and to evaluate the need for retrieval. The parameters are considered with respect to the disciplines of geomechanics, geology, hydrology, and geochemistry and are rank ordered in terms of importance. The specific role of each parameter, specific factors affecting the measurement of each parameter, and the interrelationships between the parameters are considered in detail.

14. DOCUMENT ANALYSIS – a. KEYWORDS/DESCRIPTORS
high-level waste
repository
tuff

b. IDENTIFIERS/OPEN-ENDED TERMS

15. AVAILABILITY STATEMENT
Unlimited

16. SECURITY CLASSIFICATION
(This page)
Unclassified
(This report)
Unclassified

17. NUMBER OF PAGES

18. PRICE

★U.S. GOVERNMENT PRINTING OFFICE:1987-181-682:60089

97